# MASTERS COURSE "MATERIALS SCIENCE AND SIMULATION"

# **MODULE DESCRIPTIONS**

January 2025

# **COURSE SCHEDULE**

| Mod | ule | Module description                        | Semester |     |      |      |      |      |  |  |
|-----|-----|---|----------|-----|------|------|------|------|--|--|
|     |     |   | WH       | CP  | 1st  | 2nd  | 3rd  | 4th  |  |  |
|     |     |   |          |     | sem. | sem. | sem. | sem. |  |  |
|     |     |   |          |     | LE   | LE   | LE   | LΕ   |  |  |
|     |     | Compulsory modules                        |          |     |      |      |      |      |  |  |
| 1   |     | Fundamental Materials Physics             | 4        | 5   | 22   |      |      |      |  |  |
| 2   |     | Thermodynamics and Statistical Mechanics  | 3        | 4   | 2 1  |      |      |      |  |  |
| 3   |     | Elements of Microstructure                | 4        | 6   | 3 1  |      |      |      |  |  |
| 4   |     | Programming Concepts in Materials Science | 4        | 6   | 22   |      |      |      |  |  |
| 5   |     | Numerical Methods in Materials Science    | 4        | 6   |      | 3 1  |      |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
| 6   |     | Fundamental option modules                |          |     |      |      |      |      |  |  |
|     |     | Fundamental Option Module 1               | 4        | 6   |      | 3 1  |      |      |  |  |
|     |     | Fundamental Option Module 2               | 4        | 6   |      | 3 1  |      |      |  |  |
|     |     | Fundamental Option Module 3               | 4        | 6   |      |      | 3 1  |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
| 7   |     | Advanced option module                    |          |     |      |      |      |      |  |  |
|     |     | Advanced Option 1                         | 4        | 6   |      | 22   |      |      |  |  |
|     |     | Advanced Option 2                         | 4        | 6   |      |      | 22   |      |  |  |
|     |     | Advanced Option 3                         | 4        | 6   |      |      | 22   |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
|     |     | General option module                     |          |     |      |      |      |      |  |  |
| 8   |     | General Option Module                     | 4        | 6   |      |      | 22   |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
|     |     | Key qualifications                        |          |     |      |      |      |      |  |  |
| 9   |     | Documenting and Communicating Science     | 4        | 6   |      |      |      |      |  |  |
|     | 9a  | Documenting and Communicating Science 1   | 2        | 3   | х    |      |      |      |  |  |
|     | 9b  | Documenting and Communicating Science 2   | 2        | 3   |      | х    |      |      |  |  |
| 10  |     | Non-technical elective or language course | 2        | 3   |      | х    |      |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
|     |     | Practical modules                         |          |     |      |      |      |      |  |  |
| 11  |     | Materials Modelling Lab                   | 4        | 6   | х    |      |      |      |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
|     |     | Research project and master thesis        |          |     |      |      |      |      |  |  |
| 12  |     | Research Project (180 h)                  |          | 6   |      |      | х    |      |  |  |
| 13  |     | Master Thesis and Seminar (900 h)         |          | 30  |      |      |      | х    |  |  |
|     |     |   |          |     |      |      |      |      |  |  |
|     |     | Sum semester weekly hours                 | 80       |     | 20   | 20   | 20   | 20   |  |  |
|     |     | Sum workload                              | 3600     |     | 900  | 900  | 900  | 900  |  |  |
|     |     | Sum of credit points                      |          | 120 | 30   | 30   | 30   | 30   |  |  |

**Note**: The title of lectures (submodules) referring to one module are typed in italic. The according weekly hours (WH) and credit points (CP) are summed in the title line of the module.

# **EXPLANATIONS**

### **Compulsory Modules**

1-5 The compulsory modules comprise the scientific focus of the programme and are therefore mandatory for every student.

- Fundamental Materials Physics (I)
- Thermodynamics and Statistical Mechanics (2)
- Elements of Microstructure (3)
- Programming Concepts in Materials Science (4)
- Numerical Methods in Materials Science (5)

## Fundamental Option Modules in Materials Science

6 Three elective modules can be chosen freely from:

2nd semester/summer term

- Quantum Mechanics in Materials Science (6.1)
- Microstructure and Mechanical Properties (6.2)
- Advanced Characterization Methods (6.3)
- Materials Informatics (6.4)
- Microstructure Evolution during Materials Processing (6.5)

## 3rd semester/winter term

- Atomistic Simulation Methods (6.6)
- Advanced Programming for Materials Science (6.7)
- Functional Materials: Properties and Modelling (6.8)

## Advanced Option Modules in Materials Science

7

Three optional modules can be chosen freely from the modules listed below (but also from the fundamental option modules listed above, see 6):

2nd semester/summer term

- Interfaces and Surfaces (7.1)
- Data-driven Materials Science Hands on (7.2)
- Introduction to Parallel- and Scientific Computing (7.3)
- Physics of Complex Phase Transitions in Solids (7.4)
- The CALPHAD Method in Thermodynamics and Diffusion (7.5)
- Fundamental Aspects of Materials Science and Engineering (7.6)
- Polymers and Shape Memory Alloys (7.7)
- Computational Plasticity (7.8)
- Engineering Ceramics and Coating Technology (7.9)
- Theory of Electronic Excitations in Materials (7.10)

## 3rd semester/winter term

- Phase-field Theory and Application (7.11)
- Multiscale Mechanics of Materials (7.12)
- Advanced Atomistic Simulation Methods (7.13)
- Computational Fracture Mechanics (7.14)

- Advanced Statistical Methods in Materials Science (7.15)
- Surface Science and Corrosion (7.16)
- Materials for Aerospace Applications (7.17)
- Introduction to 3-Dimensional Materials Characterization Techniques (7.18)
- Application and Implementation of Electronic Structure Methods (7.19)
- Lattice Boltzmann Modelling: From Simple Flows to Interface Driven Phenomena (7.20)
- Interatomic Potentials (7.21)

#### **General Option Module**

8 Any module from any of RUB's master's programmes will be recognized. A selection of courses offered is listed under points 6 and 7 (Elective and Specialization Modules in MS). Courses from the RUB's main course catalogue and from the international course catalogue can be taken into account. It is also possible to take a six-week industrial internship (8.1).

#### **Key Qualifications**

- 9 The Key Qualification module 9 is devided into two parts, Documenting and Communicating Science 1 (1st semester) and Documenting and Communicating Science 2 (2nd semester).
- 10This non-technical elective module should be chosen from the key qualifications offers like German language for foreigners, Project and Quality<br/>Management, Business Skills, Intercultural Competence etc.

#### **Practical Module**

11 Materials Modelling Lab: 4-5 block lectures, introduction of methods, including practical demonstration, followed by hands-on blocks.

#### **Scientific Theses**

12, 13 The research project and the master thesis with seminar represent practical self-guided research and make up 30% of all credit points.

# **EXAMINATIONS, CREDITS AND GRADES**

Each module is usually assessed by one final examination, which defines the grade for this module and is the prerequisite for credit point allocation. Module 9 spans over two semesters with two examinations, each at the end of the corresponding term.

Credit points are allocated in accordance with the students' work load comprising classes and preparation time for classes and assignments. The work load makes up the double or triple amount of the instructional contact time, depending on the degree of difficulty of the class. Together with the results of written and oral examinations as well as of practical exercises (if applicable) they form the basis for the final module grade. Since the Master's course puts an emphasis on practical research in the project report and the Master's thesis the results of these two assignments count for 30% of the total grade. The total grade is derived according to the average of all allocated module credits.

| Semester                              | 1  | 2  | 3  | 4  | Σ   |
|---------------------------------------|----|----|----|----|-----|
| Compulsory modules: 1, 2, 3, 4, 5, 11 | 27 | 6  | 0  |    | 33  |
| Option modules: 6, 7, 8               | 0  | 18 | 24 |    | 42  |
| Key qualifications: modules 9, 10     | 3  | 6  |    |    | 9   |
| Research project: module 12           |    |    | 6  |    | 6   |
| Master's thesis: module 13            |    |    |    | 30 | 30  |
| Σ                                     | 30 | 30 | 30 | 30 | 120 |

#### CREDIT ALLOCATION

Credits are allocated according the the following scheme:

| • | Compulsory                           | 33 CP = 28% |
|---|--------------------------------------|-------------|
| • | Option                               | 42 CP = 35% |
| • | Key qualifications                   | 9 CP = 7%   |
| • | Research project and Master's thesis | 36 CP = 30% |

## **DE-REGISTRATION FROM EXAMS**

The current examination regulations allow to withdraw from examination registrations.

In the case of compulsory modules (I-5, II), the withdrawal must be made in written form, stating valid reasons. Deregistration from elective and compulsory elective modules must also be made in written form, but without giving reasons, up to I week before the examination date.

Valid reasons include, for example:

• Illness of the candidate. In this case, a doctor's certificate and, in cases of doubt, a certificate from a medical officer of the RUB must also be submitted.

• The illness of a child or person to be cared for mainly alone is equivalent to the illness of the candidate.

• The examination board decides on further valid reasons.

# MODULE SCHEME AND CREDITS

| Semester I  | Semester II                                      | Sen                              | nester III        | Semester IV                             |
|---|--|----------------------------------|-------------------|---|
| Fundamental<br>Materials Physics<br>(5 CP)            | Numerical Methods<br>Materials Science<br>(6 CP) | in Fundame<br>Option M<br>(6 CP) | ental<br>Iodule 3 | Master Thesis<br>and Seminar<br>(30 CP) |
| Thermodynamics and<br>Statistical Mechanics<br>(4 CP) | Fundamental<br>Option Module 1                   | Advance<br>Option M              | d<br>Iodule 2     |   |
| Elements of<br>Microstructure                         | (0 CP)   | (8 CP)                           |                   |   |
| (6 CP)  | Fundamental<br>Option Module 2                   | Advance<br>Option M              | d<br>Iodule 3     |   |
| Programming Concepts<br>in Materials Science          | (0 CP)   | (6 CP)                           |                   |   |
| (6 CP)  | Advanced<br>Option Module 1                      | General<br>Option M              | lodule            |   |
| Materials<br>Modelling Lab                            | (6 CP)   | (6 CP)                           |                   |   |
| (6 CP)  | Docum. and Commu<br>Science 2 (3 CP)             | n.<br>Researcl<br>(6 CP)         | h Project         |   |
| Docum. and Commun.<br>Science 1 (3 CP)                | RUB Soft Skills<br>(e.g. German) (3 CP)          |                                  |                   |   |
|   | Fundamental                                      | Advanced                         | Research Projec   | Non Technical                           |
| Compulsory Module                                     | Option Module                                    | Option Module                    | and Master Thes   | is Module                               |

Course scheme: the size of the fields represents the allocated credit points.

# ALL MODULES

| FUNDAMENTAL MATERIALS PHYSICS |   |                        |                 |                 |                      |                        |         |                   |  |  |
|-------------------------------|---|------------------------|-----------------|-----------------|----------------------|------------------------|---------|-------------------|--|--|
| Mod                           | Module code         Student work-         Credits         Semester         Frequency         Duration |                        |                 |                 |                      |                        |         |                   |  |  |
|                               | 1   | load                   | 5 ECTS          | 1st             |                      | winter term            |         | 1 semester        |  |  |
|                               |   | 150 hours              |                 |                 |                      |                        |         |                   |  |  |
| 1                             | Types of c  | courses                | Contact l       | nours           | Ind                  | lependent study        | Clas    | s size            |  |  |
|                               | a) lecture  |                        | a) 30 hrs       | (2 SWS)         | 90 hours 30 students |                        |         | tudents           |  |  |
|                               | b) class  |                        | b) 30 hrs       | (2 SWS)         |                      |                        |         |                   |  |  |
| 2                             | Learning  | outcomes               |                 |                 |                      |                        |         |                   |  |  |
|                               | On succes   | ssful completion o     | f this module   | e, students re  | call t               | the connections bet    | ween    | electronic struc- |  |  |
|                               | ture, atomic bonds and macroscopic physical and mechanical properties of solids. The students can     |                        |                 |                 |                      |                        |         |                   |  |  |
|                               | classify materials according to their phenotypical properties and atomic structures. They can analyze |                        |                 |                 |                      |                        |         | Гhey can analyze  |  |  |
|                               | simple tas  | sks on material beh    | avior under a   | pplied electri  | c, ma                | agnetic, electromagi   | netic,  | thermal and me-   |  |  |
|                               | chanical f  | fields and create so   | olutions base   | d on their ur   | nders                | standing of the rela   | tions   | between atomic    |  |  |
|                               | interaction   | ns and macroscopi      | c behavior.     |                 |                      |                        |         |                   |  |  |
| 3                             | Subject ai  | ms                     |                 |                 |                      |                        |         |                   |  |  |
|                               | • I:  | ntroduction to qua     | ntum mechai     | nics and wave   | e fun                | ctions, many-electro   | on sys  | stems             |  |  |
|                               | • A   | tomic orbitals, cov    | alent and ion   | ic bonds, elec  | ctron                | gas and metallic bo    | onds    |                   |  |  |
|                               | • B   | and structure, con     | ductors, sem    | i-conductors,   | insu                 | lators, electronic tra | anspo   | rt                |  |  |
|                               | • E   | lectrical and optica   | l properties    |                 |                      |                        |         |                   |  |  |
|                               | • N   | Aagnetism, electro     | n spin, eleme   | ntary magnet    | tic m                | oments                 |         |                   |  |  |
|                               | • S   | tress and strain ter   | nsors, Hooke    | 's law and ato  | mic                  | interaction, mechan    | nical e | equilibrium       |  |  |
|                               | • N   | /letals: crystal struc | ture, strength  | n, equivalent : | stres                | S                      |         | -                 |  |  |
|                               | • P   | olymers: molecula      | r structure, n  | nechanical an   | d ph                 | ysical properties      |         |                   |  |  |
|                               | • (   | Ceramics and glass     | es, including   | semi-conduc     | tors:                | atomic structure, n    | necha   | nical and physi-  |  |  |
|                               | С   | al properties          | -               |                 |                      |                        |         | 1                 |  |  |
| 4                             | Teaching  | methods                |                 |                 |                      |                        |         |                   |  |  |
|                               | lecture, in   | cluding classes wi     | th practical ap | oplication of t | heor                 | etical content         |         |                   |  |  |
| 5                             | Prerequis   | ites for participation | n               |                 |                      |                        |         |                   |  |  |
|                               | None  |                        |                 |                 |                      |                        |         |                   |  |  |
| 6                             | Assessme  | ent methods            |                 |                 |                      |                        |         |                   |  |  |
|                               | Written e   | xamination (2 hour     | rs). Bonus po   | ints can be ga  | inec                 | l by providing soluti  | ions to | o the problem     |  |  |
|                               | sheets in   | classes.               |                 |                 |                      |                        |         |                   |  |  |
| 7                             | Prerequis   | ites for the assignr   | nent of credit  | points          |                      |                        |         |                   |  |  |
|                               | Passing th  | ne written examina     | tion (bonus p   | oints will be   | take                 | n into account)        |         |                   |  |  |
| 8                             | This mod  | ule is used in the f   | ollowing deg    | ree programn    | nes a                | s well                 |         |                   |  |  |
|                               | None  |                        |                 |                 |                      |                        |         |                   |  |  |
| 9                             | Impact of   | grade on total grad    | de              |                 |                      |                        |         |                   |  |  |
|                               | 5/117   |                        |                 |                 |                      |                        |         |                   |  |  |
| 10                            | Responsil   | bility for module      |                 |                 |                      |                        |         |                   |  |  |
|                               | Prof. Dr. A   | Alexander Hartmai      | ier             |                 |                      |                        |         |                   |  |  |
| 11                            | Other info  | ormation               |                 |                 |                      |                        |         |                   |  |  |
|                               | Moodle co   | ourse with lecture i   | notes and add   | litional mater  | ials                 |                        |         |                   |  |  |



| THE | THERMODYNAMICS AND STATISTICAL MECHANICS |                        |   |   |               |                               |              |                         |  |  |  |
|-----|--|------------------------|---|---|---------------|-------------------------------|--------------|-------------------------|--|--|--|
| Mod | ule code                                 | Student                | Credits   | Semeste   | r             | Frequency                     |              | Duration                |  |  |  |
|     | 2  | workload               | 4 ECTS  | 1st   |               | winter term                   |              | 1 semester              |  |  |  |
| _   |  | 120 hours              |   |   | Ŧ             | 1 1 1                         | <b>C</b> 1   | •                       |  |  |  |
| 1   | Types of o                               | courses:               | contact he  | DUIS  | 1nc           | dependent study               |              | ss size                 |  |  |  |
|     | a) lecture                               | 2                      | a) $50 \text{ mrs}$ (   | 2 SWS   | /3            | nours                         | 30 8         | students                |  |  |  |
| 2   | D) Class                                 | outcomog               | 0) 13 1118 (  | 13w3j   |               |                               |              |                         |  |  |  |
| 2   | Students                                 | remember the basi      | c laws of therm   | odvnamics   | the           | rmodynamic potenti            | ials a       | nd concepts such        |  |  |  |
|     | as phase of                              | coexistence, phase     | transitions and   | ransitions and phase diagrams. They combine this knowledge with the |               |                               |              |                         |  |  |  |
|     | variationa                               | l principle to cons    | ruct simple models of the temporal and spatial evolution of thermody- |   |               |                               |              |                         |  |  |  |
|     | namic pro                                | operties of solids, e  | e.g., alloys and  | magnetic n  | iatei         | rials. Moreover, the          | stude        | ents apply funda-       |  |  |  |
|     | mental co                                | oncepts of statistic   | al mechanics t  | o put such  | basi          | c models on a micr            | oscoj        | pic footing. They       |  |  |  |
|     | discuss a                                | pproximations invo     | olved in these 1  | models and  | syst          | ematically propose i          | impr         | ovements for the        |  |  |  |
| -   | individua                                | l steps.               |   |   |               |                               |              |                         |  |  |  |
| 3   | Subject a                                | ims                    | 1   | 1   |               | han an Cibba alaanaa          |              |                         |  |  |  |
|     |  | rame                   | nermodynami   | cs, phase co  | exist         | tence, Gibbs phase r          | uie a        | na phase dia-           |  |  |  |
|     | 9<br>• F                                 | Guistion of state of   | ideal cases and   | 1 extension   | tow           | ards the van-der-W/a          | ale th       | eory                    |  |  |  |
|     | • 1                                      | andau theory and       | variational prin  | icinle (Ginz  | 0117          | rg-I andaii)                  | ais tii      | leory                   |  |  |  |
|     | • 5                                      | Statistical theory of  | ideal gases lat   | tice gases at   | nd th         | regular solution th           | heory        | for thermody-           |  |  |  |
|     | n  | namic properties of    | gases and soli  | d allovs  | 14 11         | ie regular solution a         | 1001)        | for thermouy            |  |  |  |
|     | • 5                                      | Statistical mechanic   | s of stress tens  | sor: The Vir  | al fo         | ormula                        |              |                         |  |  |  |
|     | • \$                                     | Statistics of quantu   | m harmonic os   | cillator and  | spec          | cific heat of solids          |              |                         |  |  |  |
|     | • S                                      | pin statistics: Para   | and ferromagi   | netism, mea   | n fie         | eld approximation fo          | or fer       | ro-magnetism            |  |  |  |
| 4   | Teaching                                 | methods                |   |   |               |                               |              |                         |  |  |  |
|     | lecture, g                               | roup work              |   |   |               |                               |              |                         |  |  |  |
| 5   | Prerequis                                | ites for participation | on  |   |               |                               |              |                         |  |  |  |
| 6   | None                                     | 1 1                    |   |   |               |                               |              |                         |  |  |  |
| 6   | Assessme                                 | ent methods            | urg) bonug po   | inte can bo   | anin          | od by providing col           | ution        | a to the problem        |  |  |  |
|     | sheets in                                | class                  | uisj, bollus po   |   | gam           | led by providing som          | unon         | is to the problem       |  |  |  |
| 7   | Prerequis                                | ites for the assign    | nent of credit r  | oints   |               |                               |              |                         |  |  |  |
| -   | passing th                               | ne exam                | I   |   |               |                               |              |                         |  |  |  |
| 8   | This mod                                 | ule is used in the f   | ollowing degre  | e programs  | as w          | vell                          |              |                         |  |  |  |
|     | None                                     |                        |   |   |               |                               |              |                         |  |  |  |
| 9   | Impact of                                | grade on total gra     | de  |   |               |                               |              |                         |  |  |  |
|     | 4/117                                    |                        |   |   |               |                               |              |                         |  |  |  |
| 10  | Responsi                                 | bility for module      |   |   |               |                               |              |                         |  |  |  |
| 11  | Prot. Dr.                                | Fathollah Varnik       |   |   |               |                               |              |                         |  |  |  |
|     | Other info                               | ormation               | ation Marlan  | C Com   | 1. C.         | otictical measures            | . L          | h amo a dura a cati a c |  |  |  |
|     | D R Carl                                 | celle Introduction +   | sucal Mechanic  | 1.8, C. Garrow  | u: St<br>nate | rials D $\Delta$ Darter $\Re$ | AIIU Ū<br>KF | Fasterling: Dhaco       |  |  |  |
|     | transform                                | ation in metals an     | d allovs  |   | uale          | iiais, D.A. ruiter &          | к.с.         | Lasicinity, rilase      |  |  |  |
| L   | uansioill                                | iacion ni niciais di   | u anoys.  |   |               |                               |              |                         |  |  |  |



| ELEMENTS OF MICROSTRUCTURE: |                        |                        |                        |                 |        |                       |        |                     |
|-----------------------------|------------------------|------------------------|------------------------|-----------------|--------|-----------------------|--------|---------------------|
| AN I                        | NTRODU                 | <b>JCTION TO MA</b>    | TERIALS                | SCIENCE         |        |                       |        |                     |
| Mod                         | ule code               | Student work-          | Credits                | Semester        | r      | Frequency             |        | Duration            |
|                             | 3                      | load                   | 6 ECTS                 | 1st             |        | winter term           |        | 1 semester          |
|                             | -                      | 180 hours              |                        |                 |        |                       |        |                     |
| 1                           | Types of o             | courses                | Contact l              | hours           | Ind    | ependent study        | Cla    | ss size             |
|                             | a) lecture             |                        | a) 45 hrs              | (3 SWS)         | 120    | hours                 | 30 s   | students            |
|                             | b) class               |                        | b) 15 hrs              | (1 SWS)         |        |                       | 15 s   | students            |
| 2 Learning outcomes         |                        |                        |                        |                 |        |                       | 1 . 1. |                     |
|                             | Students               | acquire the basic c    | oncepts requ           | ired to under   | stanc  | 1 microstructures of  | t mai  | terials, and to ap- |
|                             | preciate 1             | their role in gove     | rning many             | important n     | nater  | als properties. In    | ey le  | earn to combine     |
|                             | and physical           | e from afferent if     | eids (chemis           | try, solid stat | e pny  | vsics, crystallograph | iy, pr | iysical chemistry   |
|                             | cossing a              | nd heat treatments     | of materials           | They also lea   | rn to  | apply this knowled    | ge to  | interpret materi    |
|                             | als proper             | ties                   | of materials.          | They also lea   | 111 10 | apply this knowled    | ge io  | merpret materi-     |
|                             | als proper             | 1105.                  |                        |                 |        |                       |        |                     |
| 3                           | Subject ai             | ims                    |                        |                 |        |                       |        |                     |
|                             | • E                    | Basics of crystallogr  | aphy, waves,           | scattering an   | d diff | fraction              |        |                     |
|                             | • (                    | Chemical bond, elas    | sticity and the        | ermal expansi   | ion    |                       |        |                     |
|                             | • [                    | Defects and interfac   | ces                    | 1               |        |                       |        |                     |
|                             | • [                    | Diffusion phenome      | nology and p           | hysics          |        |                       |        |                     |
|                             | • E                    | Basics of thermody     | namics and p           | hase transfor   | matio  | ons                   |        |                     |
|                             | • F                    | hase diagram           | -                      |                 |        |                       |        |                     |
|                             | • S                    | olidification and ti   | me-temperat            | ure-transforn   | natioi | n (TTT) diagrams      |        |                     |
|                             | • F                    | Precipitation streng   | thening                |                 |        |                       |        |                     |
|                             | • (                    | Order and disorder     | transformatio          | on              |        |                       |        |                     |
|                             | • N                    | Aartensite, pearlite   | , bainite in st        | eels            |        |                       |        |                     |
|                             | • S                    | Shape memory allo      | ys                     |                 |        |                       |        |                     |
|                             | • E                    | Brittle and ductile n  | naterials beha         | avior           |        |                       |        |                     |
|                             |                        |                        |                        |                 |        |                       |        |                     |
| 4                           | Teaching               | methods                |                        |                 |        |                       |        |                     |
| _                           | lecture, cl            | ass                    |                        |                 |        |                       |        |                     |
| 5                           | Prerequis              | ites for participation | n                      |                 |        |                       |        |                     |
| (                           | None                   |                        |                        |                 |        |                       |        |                     |
| 6                           | Assessme<br>Writton of | ent methods            |                        |                 |        |                       |        |                     |
| 7                           | Broroquia              | ites for the assign    | is).<br>nont of crodit | nointa          |        |                       |        |                     |
| /                           | Passing t              | he written examina     | tion                   | points          |        |                       |        |                     |
| 8                           | This mod               | ule is used in the f   | ollowing deg           | ree programn    | nes a  | s well                |        |                     |
| Ū.                          | none                   |                        |                        | ree heegen      | 100 u  | 5 11 012              |        |                     |
| 9                           | Impact of              | grade on total grad    | le                     |                 |        |                       |        |                     |
|                             | 6/117                  | <b>. . .</b>           |                        |                 |        |                       |        |                     |
| 10                          | Responsi               | bility for module      |                        |                 |        |                       |        |                     |
|                             | G. Eggler              | , T. Li                |                        |                 |        |                       |        |                     |
| 11                          | Other inf              | ormation               |                        |                 |        |                       |        |                     |
|                             | Literature             | , lecture script, Mo   | odle course,           | etc.            |        |                       |        |                     |





| PRO | PROGRAMMING CONCEPTS IN MATERIALS SCIENCE |                             |                               |                  |                 |                       |         |                  |  |  |
|-----|---|-----------------------------|-------------------------------|------------------|-----------------|-----------------------|---------|------------------|--|--|
| Mod | lule code                                 | Student work-               | Credits                       | Semester         | ,               | Frequency             |         | Duration         |  |  |
|     | 4   | load                        | 6 ECTS                        | 1st              |                 | winter term           |         | 1 semester       |  |  |
| 1   | Types of                                  | 180 hours                   | Contact                       | hours            | Ind             | lopondont study       | Class   | s sizo           |  |  |
| 1   | Lecture w                                 | ith integrated prac         | = 60  hrs (4)                 | SW/S)            | 120             | ) hours               | 30 st   | s size           |  |  |
|     | tical hand                                | ls-on                       | 00 1115 (1                    | 5 ( 6)           | 120             | 110415                | 50 50   | luuentis         |  |  |
| 2   | Learning                                  | outcomes                    |                               |                  |                 |                       |         |                  |  |  |
|     | On succes                                 | ssful completion o          | f this module                 | the students     | recal           | ll the basic concepts | of cor  | mputers, operat- |  |  |
|     | ing syster                                | ms. They analyse,           | write and tes                 | t Python lang    | uage            | e programs of mod     | erate o | complexity. Fur- |  |  |
|     | thermore                                  | , they have the abil        | ity to work wi                | th code editor   | s an            | d programming too     | ls and  | to program and   |  |  |
|     | to solve b                                | pasic numerical pr          | oblems in the                 | e context of o   | ther            | modules, in partic    | ular p  | roject work and  |  |  |
|     | Master th                                 | esis. The students          | will transfer                 | materials sci    | ence            | problems into an a    | bstrac  | t algorithm and  |  |  |
| 2   | implemen                                  | nt this algorithm in        | ito the taught                | structured p     | ogra            | amming language.      |         |                  |  |  |
| 5   | Subject an                                | ims<br>induction to princip | plag of comp                  | torg and ano     | otin            | a guatoma (Linuw)     |         |                  |  |  |
|     | • Intr                                    | oduction to princi          | orn programs                  | ning languag     | aung            | g systems (Linux)     |         |                  |  |  |
|     | <ul> <li>Intr</li> </ul>                  | oduction to releva          | etti programi<br>at mathemati | cal and graph    | e (ry<br>ical ( | software              |         |                  |  |  |
|     | • Frai                                    | mples that will gai         | n an overview                 | of modern n      | roor            | amming approache      | s and t | tools will       |  |  |
|     | com                                       | inples that will gan        |                               | or modern p      | logia           | amming approache.     | s and t |                  |  |  |
|     | • (                                       | data interpolation a        | and fitting                   |                  |                 |                       |         |                  |  |  |
|     | • 1                                       | linear algebra              |                               |                  |                 |                       |         |                  |  |  |
|     | • 1                                       | numerical integrat          | ion                           |                  |                 |                       |         |                  |  |  |
|     | • 1                                       | numerical solution          | of ordinary a                 | nd partial dif   | ferer           | ntial equations       |         |                  |  |  |
| 4   | Teaching                                  | methods                     |                               |                  |                 |                       |         |                  |  |  |
|     | Lecture w                                 | rith integrated han         | ds-on comput                  | er exercises v   | vith 1          | Python and Jupyter    | noteb   | ook              |  |  |
| 5   | Prerequis                                 | ites for participation      | on                            |                  |                 |                       |         |                  |  |  |
| -   | None                                      | <u> </u>                    |                               |                  |                 |                       |         |                  |  |  |
| 6   | Assessme                                  | ent methods                 |                               |                  |                 |                       |         |                  |  |  |
| 7   | Written e                                 | ites for the assign         | rs).<br>nont of crodit        | nointa           |                 |                       |         |                  |  |  |
| /   | Passing th                                | he written examina          | ition                         | points           |                 |                       |         |                  |  |  |
| 8   | This mod                                  | ule is used in the f        | following deg                 | ree programn     | 165.2           | s well                |         |                  |  |  |
| Ũ   | none                                      | uie is used in the i        | onowing degi                  | ree programm     | ics u           |                       |         |                  |  |  |
| 9   | Impact of                                 | grade on total gra          | de                            |                  |                 |                       |         |                  |  |  |
|     | 6/117                                     | 0 0                         |                               |                  |                 |                       |         |                  |  |  |
| 10  | Responsi                                  | bility for module           |                               |                  |                 |                       |         |                  |  |  |
|     | PD Dr. ha                                 | abil. Thomas Ham            | merschmidt,                   | Prof. Dr. God    | ehar            | rd Sutmann            |         |                  |  |  |
| 11  | Other info                                | ormation                    |                               |                  |                 |                       |         |                  |  |  |
|     | An online                                 | repository provide          | s Lecture not                 | es (lecture file | s and           | d video material), so | urce co | ode of programs  |  |  |
|     | which are                                 | discussed and dev           | eloped during                 | g the class and  | l exe           | rcises with solution  | s. The  | book "A primer   |  |  |
|     | on scienti                                | tic programming v           | with Python"                  | by Hans Pette    | er La           | ngtangen will be co   | vered.  |                  |  |  |



| NUMERICAL METHODS IN MATERIALS SCIENCE                 |             |                        |                   |                 |        |                        |          |                    |
|--|-------------|------------------------|-------------------|-----------------|--------|------------------------|----------|--------------------|
| Module codeStudent work-CreditsSemesterFrequencyDurate |             |                        |                   |                 |        | Duration               |          |                    |
|  | 5           | load                   | 6 ECTS            | 2nd             |        | summer term            |          | 1 semester         |
|  |             | 180 hours              |                   |                 |        |                        |          |                    |
| 1  | Types of c  | courses                | Contact           | hours           | Inc    | lependent study        | Cla      | ss size            |
|  | a) lecture  |                        | a) 45 hrs         | (3 SWS)         | 120    | ) hours                | a) 3     | 30 students        |
|  | b) class    |                        | b) 15 hrs         | (1 SWS)         |        |                        | b) 3     | 30 students        |
| 2  | Learning    | outcomes               |                   |                 |        |                        |          |                    |
|  | Students    | will remember the      | basic principl    | es of solving   | num    | erical problems in n   | nater    | ials science. They |
|  | memorize    | e the numerical sol    | lution strategi   | les for differe | nt pr  | oblems and are able    | e to a   | nalyse, select and |
|  | apply app   | ropriate numerica      | l strategies fo   | r a wide vari   | ety o  | f numerical modell     | ing t    | asks in materials  |
|  | science, fr | com the electronic s   | structure to co   | ontinua. The s  | stude  | ents appraise the uni  | fied,    | holistic approach  |
|  | to materia  | ls simulation which    | ch is not cente   | ered on or lin  | nited  | to a particular leng   | th sca   | ale. Furthermore,  |
|  | the studer  | nts assess and eval    | luate given nı    | umerical prot   | olem   | s in materials scien   | ce ar    | nd devise and im-  |
|  | plement c   | ptimal solutions.      |                   |                 |        |                        |          |                    |
| 3  | Subject ai  | ms                     |                   |                 |        |                        |          |                    |
|  | Numerica    | l methods are the      | foundation of     | f materials sin | nula   | tion and necessary     | for th   | ne implementa-     |
|  | tion of ma  | aterials theory and    | its application   | n to practical  | prob   | olems. The principle   | s of 1   | numerical meth-    |
|  | ods are in  | dependent of leng      | th scale, i.e. tl | ne solutions o  | of ele | ectronic, atomistic, r | nicro    | structural and     |
|  | continuur   | n problems often f     | follow closely    | related strate  | gies.  | . In this course the f | ocus     | is on numerical    |
|  | problems    | and challenges in      | materials scie    | ence. Applica   | tions  | s to different length  | scale    | es are introduced  |
|  | by way of   | example.               |                   |                 |        |                        |          |                    |
|  | •           | Basics: Different      | iation and int    | egration, vect  | ors a  | and tensors, product   | ts and   | d norms, series    |
|  |             | expansions             |                   |                 |        |                        |          |                    |
|  | •           | Partial differentia    | al equations: I   | Numerical int   | tegra  | ition for electrons, a | toms     | s and continuum    |
|  |             | models                 |                   | 11              | ,      | 1                      | 1.00     |                    |
|  | •           | Variational calcu      | lus: Function     | al derivatives  | and    | derivation of partial  | diffe    | erential           |
|  |             | Optimization: Or       | timization /m     | oot finding of  | ~~~**  | hma mathada far a      | :        | voluo problema     |
|  | •           | Degragation and g      | totictical anal   | Dot Infung an   | gorii  | nins, methods for e    | igen<br> | value problems     |
| 4  | Tooching    | methoda                | latistical allal  | ysis. Data alla | ilysis | s, error estimates, ir | IdCIII   | ne learning        |
| 4  | Lectures    | classes                |                   |                 |        |                        |          |                    |
| 5  | Droroquis   | ites for participation | n n               |                 |        |                        |          |                    |
| 5  | None        | nes for participation  | )II               |                 |        |                        |          |                    |
| 6  | Assessme    | ent methods            |                   |                 |        |                        |          |                    |
| Ŭ  | Written er  | xamination (2 hour     | rs). Bonus po     | ints can be ga  | inec   | l by presenting solu   | tions    | to the work-       |
|  | sheets in   | class.                 | ioji zendo pe     | into cuir de Be |        | , of presenting series |          |                    |
| 7  | Prerequis   | ites for the assign    | nent of credit    | points          |        |                        |          |                    |
| -  | Passing th  | ne written examina     | ition             | r               |        |                        |          |                    |
| 8  | This mod    | ule is used in the f   | ollowing deg      | ree programn    | nes a  | ıs well                |          |                    |
|  | none        |                        | 0 0               | 1 0             |        |                        |          |                    |
| 9  | Impact of   | grade on total gra     | de                |                 |        |                        |          |                    |
|  | 6/117       |                        |                   |                 |        |                        |          |                    |
| 10   | Responsil   | oility for module      |                   |                 |        |                        |          |                    |
|  | Prof. Dr.   | Ralf Drautz            |                   |                 |        |                        | <u> </u> |                    |
| 11   | Other info  | ormation               |                   |                 |        |                        |          |                    |
|  | Recomme     | ended literature wi    | ll be announc     | ed in class.    |        |                        |          |                    |



| QUANTUM MECHANICS IN MATERIALS SCIENCE  |  |                              |                   |               |        |                        |                   |                  |  |  |
|---|--|------------------------------|-------------------|---------------|--------|------------------------|-------------------|------------------|--|--|
| Module code         Student         Credits         Semester         Frequency         Duration |  |                              |                   |               |        |                        |                   | Duration         |  |  |
|   | 6.1  | workload                     | 6 ECTS            | 2nd           |        | summer term            |                   | 1 semester       |  |  |
|   | r  | 180 hours                    |                   |               |        |                        |                   |                  |  |  |
| 1   | Types of o   | courses:                     | Contact he        | ours          | Inc    | lependent study        | Clas              | s size           |  |  |
|   | a) lecture   |                              | a) 45 hrs (       | 3 SWS)        | 120    | ) hours a              |                   | 0 students       |  |  |
|   | b) class   |                              | b) 15 hrs (       | 1 SWS)        |        |                        | b) 10             | 0-15 students    |  |  |
| 2   | Learning   | outcomes                     | 1 6 1             |               |        |                        |                   |                  |  |  |
|   | Students   | are able to classify         | the fundament     | tals and the  | appl   | ication of quantum     | mech              | anics in materi- |  |  |
|   | als scienc   | e. They are able to          | understand tex    | tbooks and    | the 1  | research literature in | n the f           | field. They un-  |  |  |
|   | derstand the principles of electronic structure calculations in materials science, in particular density |                              |                   |               |        |                        | articular density |                  |  |  |
|   | functiona  | I theory, and their          | limitations, an   | d also gain i | nsig   | ht into the numeric    | al imp            | plementation of  |  |  |
|   | electronic   | structure method             | s. The students   | can relate e  | electi | ronic structure prop   | erties            | to the crystal   |  |  |
| 2   | structure  | and other properti           | es of materials.  | •             |        |                        |                   |                  |  |  |
| 3   | Subject an   | ims                          |                   |               |        |                        |                   |                  |  |  |
|   | • 5  | chrodinger equation          | on<br>1           |               |        |                        |                   |                  |  |  |
|   | • •  | Many-electron prob           | lem               |               |        |                        |                   |                  |  |  |
|   | • •  | Hartree/Hartree-Fo           | CK                |               |        |                        |                   |                  |  |  |
|   | • [  | Density-functional           | theory            |               |        | 1 1                    |                   |                  |  |  |
|   | • (  | Overview of basis se         | ets, plane wave   | s vs local or | bitals | s, pseudopotentials    |                   |                  |  |  |
|   | • E  | and structure, syn           | imetry groups,    | density of s  | states | 5                      |                   |                  |  |  |
|   | • 1  | Magnetism                    |                   |               |        |                        |                   |                  |  |  |
|   | • 1  | ight-binding appro           | oximation         | 1 1.1         |        |                        |                   | 1 . 1            |  |  |
|   | • 5  | selected application         | is for molecule   | s and solids  | , 1NC  | luding semiconduct     | tors ai           | nd metals        |  |  |
| 4   | Teaching   | methods                      |                   |               |        |                        |                   |                  |  |  |
| -   | lecture, cl  | ass<br>iter for nontining ti |                   |               |        |                        |                   |                  |  |  |
| 5   | Nono   | ites for participatio        | n                 |               |        |                        |                   |                  |  |  |
| 6   | Accord   | nt mathada                   |                   |               |        |                        |                   |                  |  |  |
| U   | written ev   | amination (2 hour            | c)                |               |        |                        |                   |                  |  |  |
| 7   | Prerequis  | ites for the assignt         | nent of credit i  | oints         |        |                        |                   |                  |  |  |
|   | Passing t  | he written examina           | tion              |               |        |                        |                   |                  |  |  |
| 8   | This mod   | ule is used in the f         | ollowing degre    | e programn    | nes a  | s well                 |                   |                  |  |  |
|   | None   |                              | 0.0               | 1.9           |        |                        |                   |                  |  |  |
| 9   | Impact of  | grade on total grad          | de                |               |        |                        |                   |                  |  |  |
|   | 6/117  |                              |                   |               |        |                        |                   |                  |  |  |
| 10  | Responsi   | bility for module            |                   |               |        |                        |                   |                  |  |  |
|   | Prof. Dr.  | Ralf Drautz                  |                   |               |        |                        |                   |                  |  |  |
| 11  | Other inf  | ormation                     |                   |               |        |                        |                   |                  |  |  |
|   | Lecture n  | otes will be provide         | ed. Relevant lite | erature will  | be di  | iscussed in the first  | lectur            | re.              |  |  |



| MICI | MICROSTRUCTURE AND MECHANICAL PROPERTIES |                                 |                  |                 |        |                          |              |                     |  |  |
|------|--|---------------------------------|------------------|-----------------|--------|--------------------------|--------------|---------------------|--|--|
| Mod  | ule code                                 | Student work-                   | Credits          | Semester        | ſ      | Frequency                |              | Duration            |  |  |
|      | 6.2                                      | load                            | 6 ECTS           | 2nd             |        | summer term              |              | 1 semester          |  |  |
|      |  | 180 hours                       |                  |                 |        |                          |              |                     |  |  |
| 1    | Types of o                               | courses                         | Contact          | hours           | Ind    | lependent study          | Cla          | ss size             |  |  |
|      | a) lecture                               |                                 | a) 45 hrs        | (3 SWS)         | 120    | ) hours                  | a) 3         | 30 students         |  |  |
|      | b) class                                 |                                 | b) 15 hrs        | (1 SWS)         |        |                          | <b>b</b> ) 1 | 15 students         |  |  |
| 2    | Learning                                 | outcomes                        |                  |                 |        |                          |              |                     |  |  |
|      | The stude                                | ents memorize the               | definitions o    | f mechanical    | equi   | librium and discuss      | s the        | ir different math-  |  |  |
|      | ematical f                               | formulations and s              | solution strate  | gies. They re   | call t | the basics ideas of th   | ie co        | oncept of strength  |  |  |
|      | for differe                              | ent materials. The              | students discu   | uss microstru   | ctura  | al principles of elast   | ic-pl        | astic deformation   |  |  |
|      | and their                                | relation to atomic l            | oonds and cry    | stal structure  | s. Th  | ey describe the define   | nitio        | n of an equivalent  |  |  |
|      | stress and                               | l apply it to solve s           | imple probler    | n for the defo  | rma    | tion of elastic-plasti   | c ma         | terials. They clas- |  |  |
|      | sify the b                               | asic hardening me               | echanisms of     | materials and   | d ap   | ply theoretical mode     | els to       | predict material    |  |  |
|      | strength o                               | of different materia            | als as function  | n of their mic  | rost   | ructural parameters      | . The        | ey analyze simple   |  |  |
|      | problems                                 | in mechanics of m               | naterials and s  | solve the resul | lting  | boundary value pro       | blem         | ns by using differ- |  |  |
|      | ent finite                               | element solvers.                |                  |                 |        |                          |              |                     |  |  |
| 3    | Subject ai                               | ms                              |                  |                 | _      |                          |              |                     |  |  |
|      | • Def                                    | initions and mathe              | ematical form    | ulations of m   | echa   | inical equilibrium       |              |                     |  |  |
|      | • The                                    | ory and application             | n of finite eler | ment analysis   | as n   | numerical tool to and    | alyze        | the deformation     |  |  |
|      | of e                                     | lastic-plastic mater            | ials under giv   | en boundary     | cone   | ditions                  |              |                     |  |  |
|      | • Con                                    | cepts of strength a             | and equivalen    | t stress in cor | ıtinu  | um plasticity            |              |                     |  |  |
|      | • Rela                                   | ations between ator             | mic bonds and    | d crystal struc | tures  | s to the elastic-plastic | : beh        | avior of materials  |  |  |
|      | • Phe                                    | nomenology and i                | microscopic o    | origin of hard  | lenir  | ıg mechanisms, inc       | ludi         | ng grain bounda-    |  |  |
|      | ries                                     | , dislocations, solic           | l solutions an   | d precipitatio  | n ha   | rdening                  |              |                     |  |  |
|      | • Mic                                    | romechanical mod                | lelling of mat   | erial propertie | es     |                          |              |                     |  |  |
| 4    | Teaching                                 | methods                         |                  |                 |        |                          |              |                     |  |  |
| -    | lecture, cl                              | asses                           |                  |                 |        |                          |              |                     |  |  |
| 5    | Prerequis                                | ites for participatio           | on               |                 |        |                          |              |                     |  |  |
| -    | None                                     | r r r r r r r r r r r r r r r r |                  |                 |        |                          |              |                     |  |  |
| 6    | Assessme                                 | ent methods                     |                  |                 |        |                          |              |                     |  |  |
| -    | Written e                                | xamination (2 hou               | rs). Bonus po    | ints can be ga  | ined   | l by providing soluti    | ons          | to the problem      |  |  |
|      | sheets in                                | classes.                        | , 1              | 0               |        | 71 0                     |              | 1                   |  |  |
| 7    | Prerequis                                | ites for the assign             | ment of credit   | t points        |        |                          |              |                     |  |  |
|      | Passing th                               | he written examina              | ation (bonus p   | oints will be   | take   | n into account)          |              |                     |  |  |
| 8    | This mod                                 | ule is used in the f            | following deg    | ree programn    | nes a  | s well                   |              |                     |  |  |
|      | none                                     |                                 | 0 0              |                 |        |                          |              |                     |  |  |
| 9    | Impact of                                | grade on total gra              | de               |                 |        |                          |              |                     |  |  |
|      | 6/117                                    |                                 |                  |                 |        |                          |              |                     |  |  |
| 10   | Responsi                                 | bility for module               |                  |                 |        |                          |              |                     |  |  |
|      | Prof. Dr. J                              | Alexander Hartma                | ier              |                 |        |                          |              |                     |  |  |
| 11   | Other info                               | ormation                        |                  |                 |        |                          |              |                     |  |  |
|      | Lecture n                                | otes are provided o             | online via Moo   | odle course.    |        |                          |              |                     |  |  |
|      | Literature                               | :                               |                  |                 |        |                          |              |                     |  |  |
|      | T.H. Cou                                 | rtney: Mechanical               | behavior of m    | aterials, (2nd  | edit   | ion) McGraw-Hill I       | nteri        | national Editions,  |  |  |
|      | Boston/U                                 | SA (2000)                       |                  |                 |        |                          |              |                     |  |  |
|      | G. Gottste                               | ein: Physical found             | lations of mat   | erials science  | , Spi  | ringer-Verlag (2004      | )            |                     |  |  |



| ADV | ADVANCED CHARACTERIZATION METHODS |                                   |                 |   |                |                        |        |                     |  |  |
|-----|-----------------------------------|-----------------------------------|-----------------|---|----------------|------------------------|--------|---------------------|--|--|
| Mod | ule code                          | Student work-                     | Credits         | Semester  | [              | Frequency              |        | Duration            |  |  |
|     | 6.3                               | load                              | 6 ECTS          | 2nd   |                | summer term            |        | 1 semester          |  |  |
|     | r                                 | 180 hours                         |                 |   |                |                        | 1      |                     |  |  |
| 1   | Types of c                        | courses                           | Contact l       | nours   | Inc            | lependent study        | Cla    | ss size             |  |  |
|     | a) lecture                        |                                   | a) 45 hrs       | (3 SWS)   | 120            | ) hours                | a) 3   | 0 students          |  |  |
|     | b) class                          |                                   | b) 15 hrs       | (1 SWS)   |                |                        | b) 3   | 30 students         |  |  |
| 2   | Learning                          | outcomes                          |                 |   |                |                        |        |                     |  |  |
|     | Students                          | understand the ba                 | sic description | c description of the structure of solids. They recall advanced crystallo- |                |                        |        |                     |  |  |
|     | graphic co                        | oncepts and have a                | equired funda   | amental know  | ledg           | ge of scattering and o | diffra | action of electron, |  |  |
|     | X-ray, syn                        | chrotron and neut                 | ron waves. T    | hey know ho   | w to           | apply the Bragg eq     | uatio  | on and the Ewald    |  |  |
|     | constructi                        | ion to understand o               | liffraction dat | a of different  | orig           | ines. They will apply  | / basi | ic concepts to two  |  |  |
|     | of the mo                         | ost important char                | acterization t  | echniques in  | ma             | terials science, SEN   | 1 an   | d TEM. For both     |  |  |
|     | methods                           | the mechanisms w                  | hich are respo  | onsible for di  | ttere          | nt types of image co   | ntra   | st will be appreci- |  |  |
|     | ated. The                         | students will also                | develop an a    | ppreciation o   | t adv          | vanced in situ meth    | ods.   | After this course   |  |  |
|     | the studer                        | its are able to fully             | appreciate the  | e scientific lite   | eratu          | ire on advanced chai   | acte   | rization methods.   |  |  |
|     | They are a                        | able to judge the u               | serumess or s   | specific meth   | oas            | with respect to them   | r pot  | ential to progress  |  |  |
| 2   | Subject of                        | technology.                       |                 |   |                |                        |        |                     |  |  |
| 5   | Subject al                        | ins<br>adjustion to smutpl        | line and amo    | mboug golide  |                |                        |        |                     |  |  |
|     | • Inu                             | rn basis crystallog               | anhic concon    | te  | ,              |                        |        |                     |  |  |
|     |                                   | ttoring and diffract              | ion of particle | $\mathbf{V}$  |                | unchrotron radiation   | 2 200  | utrong and aloc     |  |  |
|     | • SCa                             | (Ching and unnact                 |                 | e waves (A-la   | y5, 5          |                        | 1, 110 | utions and elec-    |  |  |
|     | • Lea                             | rn basic interpretat              | ion of diffrac  | tion regults (  | nnl            | ing Bragg equation     | Ew     | ald construction    |  |  |
|     | • LCa                             | icture factor: interr             | reting diffrac  | ted intensitie  | appi)<br>NG PY | tra spots              | , L W  | aid construction,   |  |  |
|     | • Lea                             | rn advanced scann                 | ing electron r  | nicroscopy (ii  | ntro           | duction secondary a    | nd h   | ack scattered       |  |  |
|     | elec                              | trons energy disp                 | ersive and wa   | ve length disi  | persi          | ve chemical analysi    | s ind  | lexing of Kikuchi   |  |  |
|     | line                              | s as a basis of orie              | ntation imagi   | ng SEM, in-s  | itu e          | xperiments in the S    | EM)    | aching of function  |  |  |
|     | • Lea                             | rn advanced transr                | nission electr  | on microscor  | ov (ir         | ntroduction, differer  | ices   | between conven-     |  |  |
|     | tion                              | al and advanced m                 | ethods – field  | d emission gu   | ins [          | FEG], high angular     | dark   | field detectors     |  |  |
|     | [HA                               | AD]), chemical an                 | alysis by EDX   | K and EELS, u   | sing           | Kikuchi lines as ma    | aps f  | or tilting experi-  |  |  |
|     | men                               | nts, apply tilting ex             | periments to    | identify cryst  | al de          | efects [focus: disloca | tions  | ], in-situ experi-  |  |  |
|     | men                               | nts in the SEM)                   |                 |   |                |                        |        |                     |  |  |
|     | • Lea                             | rn to appreciate ot               | her importan    | t advanced cl   | iarac          | cterization methods    | (brie  | ef introduction to  |  |  |
|     | ator                              | m probe analysis at               | nd high resolu  | ution transmi   | issio          | n electron microsco    | py)    |                     |  |  |
|     |                                   | .1 1                              |                 |   |                |                        |        |                     |  |  |
| 4   | lecture                           | methods                           |                 |   |                |                        |        |                     |  |  |
| 5   | Droroquis                         | ass, lau<br>ites for participatic | n               |   |                |                        |        |                     |  |  |
| 5   | successful                        | l completion of "Fl               | ements of Mi    | crostructure'   | , (J)          | or equivalent          |        |                     |  |  |
| 6   | Assessme                          | nt methods                        | cificints of Mi | leiostructure   | (2)            |                        |        |                     |  |  |
| Ŭ   | written ex                        | amination (2 hour                 | S)              |   |                |                        |        |                     |  |  |
| 7   | Prerequis                         | ites for the assignr              | nent of credit  | points  |                |                        |        |                     |  |  |
| -   | passing th                        | ne written examina                | tion            | <b>r</b>  |                |                        |        |                     |  |  |
| 8   | This mod                          | ule is used in the f              | ollowing degr   | ree programn  | nes a          | s well                 |        |                     |  |  |
|     | Master of                         | Science in Mecha                  | nical Enginee   | ring: Werksto   | off- a         | nd Microengineerir     | ıg     |                     |  |  |
| 9   | Impact of                         | grade on total grad               | le              | 0   |                | 0                      | 0      |                     |  |  |
|     | 6/117                             | 0                                 |                 |   |                |                        |        |                     |  |  |
| 10  | Responsil                         | bility for module                 |                 |   |                |                        |        |                     |  |  |
|     | Prof. Dr                          | Ing. Jan Frenzel, P               | rof. Dr. Tong   | Li  |                |                        |        |                     |  |  |
| 11  | Other info                        | ormation                          | 0               |   |                |                        |        |                     |  |  |
|     | A list with                       | n recommended lit                 | erature and cl  | lass notes is a   | vaila          | able online.           |        |                     |  |  |



| MATERIALS INFORMATICS |   |  |   |   |  |   |   |   |  |
|-----------------------|---|--|---|---|--|---|---|---|--|
| Mod                   | lule code   | Student work-  | Credits   | Semester  | r  | Frequency   |   | Duration  |  |
|                       | 6.4   | load   | 6 ECTS  | 2nd   |  | summer term   |   | 1 semester  |  |
| -                     |   | 180 hours  | <u> </u>  |   | <b>.</b>                                 | 1 1 1   | <b>C1</b>                                     |   |  |
| 1                     | Types of o  | courses  | Contact I   | 1000  |  | lependent study   | a) 30 students                                |   |  |
|                       | a) lecture  |  | a) $30 \text{ hrs}$   | a) $50 \text{ mrs} (2.5 \text{ s}\text{ s}) = 1$<br>b) $30 \text{ hrs} (2.5 \text{ s}\text{ s}\text{ s})$ |  | ) nours   | a) 3  | 30 students   |  |
| 2                     | D) Class  | outcom og  | D) 50 ms  | (2 5 W 5)   |  |   | U) 1  | 5 students  |  |
| 3                     | After succ<br>materials<br>ful studer<br>learning r<br>materials<br>"workflow   | cessful completion<br>science. They can a<br>nts are able to judge<br>method to solve a p<br>science by implem<br>v" in written and pr | of the modul<br>assess quality<br>the applicab<br>roblem in ma<br>entation in P<br>resentation fo | e students ar<br>and dimensi<br>ility and choo<br>aterials science<br>ython code a<br>orm.                | e abl<br>ions<br>ose a<br>ce. T<br>nd ca | e to explain the imp<br>of materials data an<br>n appropriate data<br>hey are able to solve<br>an document, visua | pact o<br>nd me<br>sciene<br>e a "d<br>lize a | f <i>informatics</i> in<br>etadata. Success-<br>ce / machine<br>ata problem" in<br>nd present a |  |
|                       | <ul> <li>From data to data science to materials informatics</li> <li>Data sources: materials data bases and how to organize data</li> <li>Combinatorics, probabilities, and statistics</li> <li>Descriptors and representations for materials: dimensions of data</li> <li>Machine learning <ul> <li>Classification and regression</li> <li>Supervised and unsupervised learning</li> <li>Dimensionality reduction</li> <li>Clustering</li> <li>Deep learning and artificial neural networks</li> </ul> </li> <li>End-to-end workflows: data, features, model, validation, application</li> </ul> |  |   |   |  |   |   |   |  |
| 4                     | <b>Teaching</b> lecture, as   | <b>methods</b><br>ssisted tutorials in (   | CIP-pool  |   |  |   |   |   |  |
| 5                     | Prerequis   | ites for participatio  | n   |   |  |   |   |   |  |
|                       | None  |  |   |   |  |   |   |   |  |
| 6                     | Assessme  | ent methods  |   |   |  |   |   |   |  |
|                       | Written e   | xam (2 hours)  |   |   |  |   |   |   |  |
| 7                     | Prerequis   | ites for the assignm   | nent of credit  | points  |  |   |   |   |  |
|                       | Passing th  | he module examina  | tion  |   |  | 11  |   |   |  |
| 8                     | This mod  | ule is used in the f   | ollowing degi   | ree programm  | nes a                                    | is well   |   |   |  |
| 0                     | None<br>Immediate (   |  | 1   |   |  |   |   |   |  |
| 9                     | 6/113   | grade on total grad  | le  |   |  |   |   |   |  |
| 10                    | Respondi  | hility for module  |   |   |  |   |   |   |  |
| 10                    | Prof Dr   | Markus Stricker  |   |   |  |   |   |   |  |
| 11                    | Other inf   | ormation   |   |   |  |   |   |   |  |
| 11                    | Suggester   | l literature:  |   |   |  |   |   |   |  |
|                       | Suggested literature:<br>Materials Data Science – An Introduction to Data Mining, Machine Learning, and Data-Driven Pre-<br>dictions for Materials Scientists; Stefan Sandfeld, Springer (2024)   |  |   |   |  |   |   |   |  |



| MIC | MICROSTRUCTURE EVOLUTION DURING MATERIALS PROCESSING                                |                         |                  |                |        |                       |          |                 |  |  |
|-----|---|-------------------------|------------------|----------------|--------|-----------------------|----------|-----------------|--|--|
| Mod | lule code   | Student                 | Credits          | Semeste        | r      | Frequency             |          | Duration        |  |  |
|     | 6.5   | workload                | 6 ECTS           | 3rd            |        | summer term           |          | 1 semester      |  |  |
|     |   | 180 hours               |                  |                |        |                       |          |                 |  |  |
| 1   | Types of o  | courses:                | Contact he       | ours           | Inc    | lependent study       | Class    | size            |  |  |
|     | a) lecture  |                         | a) 30 hrs (1     | 2 SWS)         | 120    | ) hours               | a) 30    | students        |  |  |
|     | b) numer  | ical exercises          | b) 30 hrs (      | 2 SWS)         |        |                       | b) 15    | students        |  |  |
| 2   | Learning  | outcomes                |                  |                |        |                       |          |                 |  |  |
|     | Students  | can explain the un      | derlying princi  | ples of the f  | inite  | element/finite volu   | me me    | ethod to solve  |  |  |
|     | problems  | in continuum me         | chanics includi  | ng phase tra   | insf   | ormations. They rec   | all mea  | an-field models |  |  |
|     | and rate e  | equation solutions.     | With the phase   | e-field meth   | od tl  | hey are able to solve | free bo  | oundary prob-   |  |  |
|     | lems couj   | pled to a thermody      | namic material   | description    | . Wi   | th the help of these  | widely   | used numeri-    |  |  |
|     | cal metho   | ods in industrial an    | d academic ma    | iterials scier | ice tl | he students can mo    | del and  | l solve materi- |  |  |
| -   | als scienc  | e problems and the      | ey can describe  | the limitati   | ons    | of these methods.     |          |                 |  |  |
| 3   | Subject aims  |                         |                  |                |        |                       |          |                 |  |  |
|     | • Introduction into Partial Differential Equation and Boundary Value Problems (BVP) |                         |                  |                |        |                       |          |                 |  |  |
|     | Principles of thermodynamics of multi-phase systems                                 |                         |                  |                |        |                       |          |                 |  |  |
|     | CALPHAD thermodynamics and kinetics of multicomponent diffusion                     |                         |                  |                |        |                       |          |                 |  |  |
|     | Mean field models of microstructure evolution                                       |                         |                  |                |        |                       |          |                 |  |  |
|     | Rate equations for precipitation including numerical integration                    |                         |                  |                |        |                       |          |                 |  |  |
|     | • (   | Concepts of non-eq      | uilibrium phas   | e transform    | atio   | ns                    |          |                 |  |  |
|     | • I   | ntroduction to free     | e boundary prol  | blems          |        |                       |          |                 |  |  |
|     | • ]   | Thermodynamic co        | ncept of the Ph  | hase-field m   | etho   | d and practical appli | ication  | S               |  |  |
| 4   | Teaching  | methods                 |                  |                |        |                       |          |                 |  |  |
|     | lecture, n  | umerical exercises      |                  |                |        |                       |          |                 |  |  |
| 5   | Prerequis   | sites for participation | on               |                |        | 1:                    |          |                 |  |  |
| (   | Dackgrou  | na in mechanical e      | engineering, pr  | lysics or rela | tea    | discipline            |          |                 |  |  |
| 0   | Assessine   | amination (2 hour       | a) Ronus poin    | ta can bo ga   | inod   | by providing coluti   | ong to t | the problem     |  |  |
|     | shoots in   | class                   | s). Donus pom    | is call be ga  | ineu   | by providing solution |          | uie problem     |  |  |
| 7   | Drerequis   | tes for the assign      | ment of credit r | oints          |        |                       |          |                 |  |  |
| 1   | nassing th  | ne written examina      | tion (bonus po   | ints will be   | akei   | n into account)       |          |                 |  |  |
| 8   | This mod  | ule is used in the f    | following degre  | e programn     | ies a  | is well               |          |                 |  |  |
| Ũ   | none  | uie is used in the i    | ono wing degre   | e programm     | 105 0  |                       |          |                 |  |  |
| 9   | Impact of grade on total grade  |                         |                  |                |        |                       |          |                 |  |  |
|     | 6/117   |                         |                  |                |        |                       |          |                 |  |  |
| 10  | Responsi  | bility for module       |                  |                |        |                       |          |                 |  |  |
|     | Prof. Dr.   | Ingo Steinbach          |                  |                |        |                       |          |                 |  |  |
| 11  | Other inf   | ormation                |                  |                |        |                       |          |                 |  |  |
|     | Lecture n   | otes are provided o     | online.          |                |        |                       |          |                 |  |  |



| ATOMISTIC SIMULATION METHODS |  |                        |                  |               |       |                       |        |                   |  |
|------------------------------|--|------------------------|------------------|---------------|-------|-----------------------|--------|-------------------|--|
| Mod                          | ule code   | Student                | Credits          | Semeste       | r     | Frequency             |        | Duration          |  |
|                              | 6.6  | workload               | 6 ECTS           | 3rd           |       | winter term           |        | 1 semester        |  |
|                              |  | 180 hours              |                  |               |       |                       |        |                   |  |
| 1                            | Types of o   | courses:               | Contact he       | ours          | Ind   | lependent study       | Cla    | ss size           |  |
|                              | a) lecture   |                        | a) 45 hrs (      | 3 SWS)        | 120   | ) hours               | a) 3   | 0 students        |  |
|                              | b) class   |                        | b) 15 hrs (      | 1 SWS)        |       |                       | b) 1   | 10-15 students    |  |
| 2                            | Learning   | outcomes               |                  |               |       |                       |        |                   |  |
|                              | Students   | recall models for th   | e interatomic    | interaction a | and   | can explain how the   | se in  | teractions can be |  |
|                              | represent  | ed by potentials. Th   | iey are able to  | apply metho   | ods s | such as molecular dy  | ynam   | nics and kinetic  |  |
|                              | Monte Ca   | rlo simulations to     | calculate the ev | volution of t | he at | tomic structure of m  | lateri | ials and the re-  |  |
|                              | sulting m  | aterial properties.    | hey can discu    | ss the impo   | rtano | ce of the time and le | ength  | scales in atomic  |  |
|                              | modelling  | g. The successful pa   | articipants will | be able to a  | pply  | atomistic simulatio   | on me  | ethods to solve   |  |
| -                            | problems   | in materials science   | e.               |               |       |                       |        |                   |  |
| 3                            | Subject aims   |                        |                  |               |       |                       |        |                   |  |
|                              | Empirical and semi-empirical potentials for ionic, covalent and metallic materials   |                        |                  |               |       |                       |        |                   |  |
|                              | • A  | Atomic dynamics        | 1.1              |               |       |                       |        |                   |  |
|                              | <ul> <li>Statistics of atomic ensembles</li> <li>Observables in atomistic simulations (MSD_RDE_specific heat and free energy)</li> </ul>                                   |                        |                  |               |       |                       |        |                   |  |
|                              | <ul> <li>Observables in atomistic simulations (MSD, RDF, specific heat and free energy)</li> <li>Monte Carle (kinetic, Metropolic) and Transition state theory.</li> </ul> |                        |                  |               |       |                       |        |                   |  |
|                              | Monte Carlo (kinetic, Metropolis) and Transition-state theory  |                        |                  |               |       |                       |        |                   |  |
|                              | • 1  | attice-gas-Hamilto     | nian (Ising-mo   | odel, cluster | expa  | ansion)               |        |                   |  |
|                              | • N  | Aagnetism (Heisen      | berg-model)      |               |       |                       |        |                   |  |
|                              | • [  | inking atomistic si    | mulations to t   | he electronic | c, m  | icrostructural and m  | lacro  | scopic models     |  |
| 4                            | Teaching   | methods                |                  |               |       |                       |        |                   |  |
| -                            | lecture, cl  | ass, problem sheet     | S                |               |       |                       |        |                   |  |
| 5                            | Prerequis  | ites for participation | n<br>Mach        | nica in Mat   |       | la Caion co"/Madula   | ( 1) : | a recommended     |  |
| 6                            | Accessio   | nt methoda             |                  |               | ena   | is science (module    | 0.1)1  | is recommended    |  |
| 0                            | writton ov   | amination (2 hour      | s) Bonus poin    | te can be ga  | inod  | by providing soluti   | one t  | o the problem     |  |
|                              | sheets in  | class                  | sj. Bollus polli | is call be ga | meu   | by providing solution | 0115 0 | o the problem     |  |
| 7                            | Prerequis  | ites for the assignm   | nent of credit i | oints         |       |                       |        |                   |  |
|                              | passing th   | ne written examina     | tion (bonus po   | ints will be  | takeı | n into account)       |        |                   |  |
| 8                            | This mod   | ule is used in the f   | ollowing degre   | e programn    | nes a | is well               |        |                   |  |
| _                            | none   |                        | 8 8              | 1.9           |       |                       |        |                   |  |
| 9                            | Impact of grade on total grade   |                        |                  |               |       |                       |        |                   |  |
|                              | 6/117  | - 0                    |                  |               |       |                       |        |                   |  |
| 10                           | Responsi   | bility for module      |                  |               |       |                       |        |                   |  |
|                              | Prof. Dr.  | Ralf Drautz            |                  |               |       |                       |        |                   |  |
| 11                           | Other info   | ormation               |                  |               |       |                       |        |                   |  |
|                              | Lecture n  | otes will be provide   | d. Relevant lite | erature will  | be di | iscussed in the first | lectu  | ire.              |  |



| ADVANCED PROGRAMMING FOR MATERIALS SCIENCE |  |                        |                     |                |       |                       |                |                      |  |
|--|--|------------------------|---------------------|----------------|-------|-----------------------|----------------|----------------------|--|
| Mod  | lule code  | Student work-          | Credits             | Semester       | r     | Frequency             |                | Duration             |  |
|  | 6.7  | load                   | 6 ECTS              | 2nd            |       | winter term           |                | 1 semester           |  |
|  |  | 180 hours              |                     |                | -     | 1 1 1                 | <b>C1</b>      |                      |  |
| 1  | Types of c   | courses                | Contact             | hours          |       | lependent study       | Cla            | ss size              |  |
|  | a) lecture   |                        | a) $30 \text{ hrs}$ | (2 SWS)        | 120   | ) nours               | a) 3           | 50 students          |  |
| 2  | D) Class   | outcom or              | b) 30 mrs           | (2 5 W 5)      |       |                       | U) 1           | 15 students          |  |
| Z  | The stude  | outcomes               | dwanced pro         | aromming to    | hni   | ning that are relevan | at for         | materials sci        |  |
|  | ence The   | w can classify diffe   | rent program        | ming languag   |       | nd are able to gener  | n iui<br>ate c | omputer code         |  |
|  | for compi  | led languages to so    | lve basic mat       | thematical an  | d nh  | vsical problems. Th   | ev 119         | se tools that facil- |  |
|  | itate code   | development and        | employ best r       | programming    | ora   | ctices. The students  | appl           | v these concepts     |  |
|  | to create a  | dvanced algorithm      | is that solve of    | omplex probl   | ems   | in materials science  | e.             | y allose colleepts   |  |
| 3  | Subject ai   | ims                    |                     |                |       |                       |                |                      |  |
|  | • Con  | npiled languages (I    | Fortran, C)         |                |       |                       |                |                      |  |
|  | • Object-oriented programming (python, C++)                |                        |                     |                |       |                       |                |                      |  |
|  | • Para   | allel programming      | C III               | ,              |       |                       |                |                      |  |
|  | • Bes  | t practices (testing,  | documentati         | ion, version c | ontro | ol)                   |                |                      |  |
|  | Advanced algorithms  |                        |                     |                |       |                       |                |                      |  |
|  | <ul> <li>Variational basis set methods for PDEs</li> </ul> |                        |                     |                |       |                       |                |                      |  |
|  | 0  | Stochastic Monte       | -Carlo metho        | ds             |       |                       |                |                      |  |
|  | 0  | Time-propagatior       | 1                   |                |       |                       |                |                      |  |
| 4  | Teaching   | methods                |                     |                |       |                       |                |                      |  |
|  | lecture, as  | ssisted tutorials in   | CIP-pool, mi        | ni-project     |       |                       |                |                      |  |
| 5  | Prerequis  | ites for participation | n                   |                |       |                       |                |                      |  |
|  | None   |                        |                     |                |       |                       |                |                      |  |
| 6  | Assessme   | ent methods            |                     |                |       |                       |                |                      |  |
|  | Portfolio  | exam including mi      | ni-project, se      | minar, and re  | eport |                       |                |                      |  |
| 7  | Prerequis  | ites for the assignr   | nent of credit      | t points       |       |                       |                |                      |  |
|  | Passing th   | ne module examina      | ation               |                |       | 11                    |                |                      |  |
| 8  | This mod   | ule is used in the f   | ollowing deg        | ree programn   | nes a | is well               |                |                      |  |
| 0  | Inone<br>Impost of   | Canada an tatal ana    | 4.0                 |                |       |                       |                |                      |  |
| 9  | 6/117  | grade on total grad    | le                  |                |       |                       |                |                      |  |
| 10   | Responsil  | bility for module      |                     |                |       |                       |                |                      |  |
| 10   | Prof. Dr   | Miguel Marques         |                     |                |       |                       |                |                      |  |
| 11   | Other info   | ormation               |                     |                |       |                       |                |                      |  |
|  | -  |                        |                     |                |       |                       |                |                      |  |
|  | 1  |                        |                     |                |       |                       |                |                      |  |



| FUNCTIONAL MATERIALS: PROPERTIES AND MODELLING |  |                       |                  |                 |  |                      |        |                    |  |
|--|--|-----------------------|------------------|-----------------|--|----------------------|--------|--------------------|--|
| Mod  | ule code   | Student               | Credits          | Semester        | t                                      | Frequency            |        | Duration           |  |
|  | 6.8  | workload              | 6 ECTS           | 3rd             |  | winter term          |        | 1 semester         |  |
|  |  | 180 hours             |                  |                 |  |                      |        |                    |  |
| 1  | Types of o   | courses               | Contact l        | hours           | Ind                                    | lependent study      | Cla    | ss size            |  |
|  | a) lecture   |                       | a) 45 hrs        | (3 SWS)         | 120                                    | ) hours              | a) 3   | 0 students         |  |
|  | b) class   |                       | b) 15 hrs        | (1 SWS)         |  |                      | b) 1   | 5 students         |  |
| 2  | Learning   | outcomes              |                  |                 |  |                      |        |                    |  |
|  | After part   | icipation in this m   | odule, studen    | its memorize    | the                                    | discussed functiona  | l pro  | perties of materi- |  |
|  | als. They  | recall and understa   | ind the under    | lying physica   | l cor                                  | cepts. Furthermore   | , the  | y can outline the  |  |
|  | challenge  | s for materials scie  | nce, and sug     | gest proper si  | mula                                   | ation methods to ad  | dress  | s these on the     |  |
|  | relevant s   | cales. They are able  | e to analyse, c  | compare and a   | apply                                  | y these concepts and | l met  | hods to current    |  |
|  | problems   | in materials science  | ce.              | 1               |  |                      |        |                    |  |
| 3  | Subject ai   | ms                    |                  |                 |  |                      |        |                    |  |
|  | This course focuses on functional materials, their relevance for application, and the interplay of   |                       |                  |                 |  |                      |        |                    |  |
|  | electronic, atomistic, microstructural and functional properties. The objectives are the fundamental |                       |                  |                 |  |                      |        |                    |  |
|  | understanding of functional responses and their degeneration through functional fatigue as well as   |                       |                  |                 |  |                      |        |                    |  |
|  | routes to optimize functional properties.  |                       |                  |                 |  |                      |        |                    |  |
|  | The main focus is on materials for energy conversion and storage, e.g.                               |                       |                  |                 |  |                      |        |                    |  |
|  | Battery materials  |                       |                  |                 |  |                      |        |                    |  |
|  | •  | Materials for capa    | citors           |                 |  |                      |        |                    |  |
|  | Permanent magnets  |                       |                  |                 |  |                      |        |                    |  |
|  | Materials for solar cells  |                       |                  |                 |  |                      |        |                    |  |
|  | •  | Magnetic, ferroele    | ctric. multife   | rroic phases a  | ınd r                                  | phase transitions    |        |                    |  |
|  | •  | Superconducting       | materials        | <b>F</b>        | 1                                      |                      |        |                    |  |
|  | In additio   | n to physical conce   | epts, the lectu  | re focuses on   | the                                    | modelling of the ma  | ateria | al properties      |  |
|  | across the   | relevant scales. W    | e will discuss   | s. compare an   | d ap                                   | ply simulations usi  | ng e.g | л.<br>Г. Г Г       |  |
|  | • \$   | pin models            |                  | , <u>-</u>      | F                                      | F-7 ~                | -00    | 5.                 |  |
|  | • T  | Pensity functional t  | heory            |                 |  |                      |        |                    |  |
|  | • 1  | Aolecular Dynamic     | s                |                 |  |                      |        |                    |  |
|  | • 1  | andau theory          |                  |                 |  |                      |        |                    |  |
| 4  | Teaching   | methods               |                  |                 |  |                      |        |                    |  |
| 1  | lecture cl   | 255                   |                  |                 |  |                      |        |                    |  |
| 5  | Prerequis  | ites for participatic | n                |                 |  |                      |        |                    |  |
| 5  | Basic kno  | wledge on quantu      | n mechanics      | / solid state r | hvsi                                   | ics is of advantage  |        |                    |  |
| 6  | Assessme   | nt methods            | ii iiiceiluilles |                 | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | les is of advantage  |        |                    |  |
| Ŭ  | Written e  | xam (2 hours): if le  | ss than 10 sti   | idents: oral e  | vam                                    | (20 minutes)         |        |                    |  |
| 7  | Prerequis  | ites for the assign   | nent of credit   | noints          | Autti                                  | Zommates             |        |                    |  |
| 1  | Passed ex  | res for the assign    | field of cicult  | points          |  |                      |        |                    |  |
| 8  | This mod   | ule is used in the f  | ollowing deg     | ree programn    | nes a                                  | s well               |        |                    |  |
| Ŭ  | -  | ule is used in the i  | onowing degi     | ice programm    | 105 u                                  |                      |        |                    |  |
| 9  | Impact of  | grade on total grad   | le               |                 |  |                      |        |                    |  |
| 1  | 6/117  | grade on total grad   | ac .             |                 |  |                      |        |                    |  |
| 10   | Responsil  | pility for module     |                  |                 |  |                      |        |                    |  |
| 1  | Prof Dr  | Anna Grünebohm        |                  |                 |  |                      |        |                    |  |
| 11   | Other info   | ormation              |                  |                 |  |                      |        |                    |  |
|  | Lecture n  | otes will be provide  | h                |                 |  |                      |        |                    |  |
|  | Lecture II   | ores will be provide  |                  |                 |  |                      |        |                    |  |





| INTERFACES AND SURFACES |   |                        |  |  |        |                        |        |                     |  |
|-------------------------|---|------------------------|--|--|--------|------------------------|--------|---------------------|--|
| Mod                     | ule code  | Student                | Credits  | Semeste  | r      | Frequency              |        | Duration            |  |
|                         | 7.1   | workload               | 6 ECTS   | 2nd  |        | summer term            |        | 1 semester          |  |
|                         |   | 180 hours              |  |  |        |                        |        |                     |  |
| 1                       | Types of o  | courses:               | Contact he   | ours   | Ind    | lependent study        | Cla    | ss size             |  |
|                         | a) lecture  |                        | a) 45 hrs (  | 3 SWS)   | 120    | ) hours                | a) 2   | 0 students          |  |
|                         | b) class  |                        | b) 15 hrs (  | 1 SWS)   |        |                        | b) 1   | l0 students         |  |
| 2                       | Learning  | outcomes               | <u> </u>   |  |        |                        |        |                     |  |
|                         | Students  | will understand th     | e relevance of s                                       | surfaces and   | inte   | rfaces in materials s  | scien  | ce and gain         |  |
|                         | basic kno   | wledge of experime     | ental and comp   | outational te  | chni   | ques to characterize   | e thei | m. They under-      |  |
|                         | stand the   | relationship betwe     | en atomistic de  | escriptions o  | of int | terfaces/surfaces an   | d ma   | croscopic mate-     |  |
|                         | rials prop  | erties, especially th  | ermodynamic  | nodynamic and mechanical properties. They will develop the skills to |        |                        |        |                     |  |
|                         | read and  | understand the rel     | evant literature                                       | , to choose t  | he n   | nost suited experime   | ental  | or modelling        |  |
|                         | approache   | es for specific tasks  | s and to applyth                                       | nem to mate  | rial s | science problems.      |        |                     |  |
| 3                       | Subject ai  | ms                     |  |  |        |                        |        |                     |  |
|                         | • I:  | ntroduction to sur     | faces and inter  | faces for opt  | ical,  | electronic, magneti    | c and  | l mechanical        |  |
|                         | p   | properties and their   | importance fo  | or materials   | desią  | gn including metals    | , sen  | niconductor, ox-    |  |
|                         | ie  | des                    |  |  |        |                        |        |                     |  |
|                         | • P   | Principles of interfa  | ce/surface crys  | stallography   | and    | indexing geometrie     | es in  | atomistic mod-      |  |
|                         | e   | ls. Introducing cla    | ssification and  | nomenclatu   | re o   | f surfaces and grain   | bou    | ndaries             |  |
|                         | • N   | Aechanisms and in      | nportance of su  | ırface relaxa  | tion   | /reconstruction and    | opti   | mization of         |  |
|                         | S   | olid-solid interface   | degrees of free  | edom   |        |                        |        |                     |  |
|                         | • E   | Empirical and there    | nodynamic mo   | dels of inter  | face   | /surface properties,   | for ]  | oure inter-         |  |
|                         | fa  | aces/surfaces as w     | ell as for intera                                      | ctions with a  | adso   | rbates, vacancies, in  | npur   | ities, and disloca- |  |
|                         | tions   |                        |  |  |        |                        |        |                     |  |
|                         | • Experimental characterization of interface/surface structures (diffraction, scanning, micros- |                        |  |  |        |                        |        |                     |  |
|                         | С   | opy, spectroscopy      | methods), plan   | ning specifi   | c exp  | periments and relate   | e exp  | erimental and       |  |
|                         | t   | heoretical results     |  |  |        |                        |        |                     |  |
|                         | • N   | Aethods for compu      | tational detern  | nination of a  | tom    | istic interface/surfa  | ce st  | ructures and        |  |
|                         | p   | roperties. Possibil    | ities and limita                                       | tions of ator  | nisti  | c models               |        |                     |  |
| 4                       | Teaching  | methods                |  |  |        |                        |        |                     |  |
| -                       | lecture, co   | iter Commentiation     |  |  |        |                        |        |                     |  |
| 5                       | booleanous  | ites for participation | n<br>nistra or relate                                  | d diaciplina   |        |                        |        |                     |  |
| 6                       | Aggaggma  | na mathada             | filstry of relate                                      | a aiscipiine   |        |                        |        |                     |  |
| 0                       | Assessine   | hours) or oral ova     | mination (0.5 k  | ourg) donor  | dine   | a on size of the class |        | nus points con      |  |
|                         | be gained   | by complementar        | v tasks distribu                                       | ted in the le  | cture  |                        | s. do  | nus points can      |  |
| 7                       | Drerequis   | ites for the assign    | nent of credit i                                       | noints   | ctur   |                        |        |                     |  |
| ·                       | nassing th  | ne evamination (bo     | nus points will  | be taken in  | to ac  | count)                 |        |                     |  |
| 8                       | This mod  | ule is used in the f   | ollowing degre   | e programn   |        | s well                 |        |                     |  |
| 0                       | none  | uic is used in the i   | onowing degre  | c programm   | ics a  | is well                |        |                     |  |
| 9                       | Impact of   | orade on total gra     | de   |  |        |                        |        |                     |  |
| ,                       | 6/117   |                        |  |  |        |                        |        |                     |  |
| 10                      | Responsi  | pility for module      |  |  |        |                        |        |                     |  |
|                         | PD Dr. ha   | ibil. Thomas Ham       | merschmidt. P  | D Dr. habil.   | Reb    | ecca Ianisch           |        |                     |  |
| 11                      | Other information   |                        |  |  |        |                        |        |                     |  |
|                         | Lecture n   | otes will be provide   | ed.  |  |        |                        |        |                     |  |
|                         | Recomme   | ended Literature:      |  |  |        |                        |        |                     |  |
|                         | I. M. Howe: Interfaces in mat   |                        | aterials, Wiley Interscience (1997);                   |  |        |                        |        |                     |  |
|                         | A. Gross:   | Theoretical surfac     | e science: A microscopic perspective, Springer (2009). |  |        |                        |        |                     |  |

| DATA-DRIVEN MATERIALS SCIENCE – HANDS ON |  |                        |                  |                |                                   |                       |        |                   |  |
|--|--|------------------------|------------------|----------------|-----------------------------------|-----------------------|--------|-------------------|--|
| Mod                                      | ule code   | Student                | Credits          | Semeste        | er                                | Frequency             |        | Duration          |  |
|  | 7.2  | workload               | 6 ECTS           | 2nd            |                                   | summer term           |        | 1 semester        |  |
|  |  | 180 hours              |                  |                |                                   |                       |        |                   |  |
| 1  | Types of c   | courses:               | Contact he       | ours           | Ind                               | lependent study       | Cla    | ss size           |  |
|  | a) lectures  | 3                      | a) 30 hrs (      | 2 SWS)         | 120                               | ) hours               | a) 2   | 0 students        |  |
|  | b) hands-  | on practical studie    | s b) 30 hrs (    | 2 SWS)         |                                   |                       | b) 2   | 20 students       |  |
| 2  | Learning   | outcomes               |                  | ,              |                                   |                       | . ,    |                   |  |
|  | After part   | icipating in the mo    | odule students   |                |                                   |                       |        |                   |  |
|  | 1  | 1 0                    |                  |                |                                   |                       |        |                   |  |
|  | • R  | Remember the basi      | c concepts of d  | ata-driven n   | nate                              | rial science          |        |                   |  |
|  | • a  | pply common data       | -driven metho    | ds of superv   | ised                              | and unsupervised l    | earni  | ng, deep learn-   |  |
|  | iı   | ng to describe and     | analyze given o  | data sets      |                                   |                       |        |                   |  |
|  | • d  | iscuss limitations     | and applicabili  | ty of these n  | neth                              | ods in the context of | f mat  | erials science    |  |
|  | а  | nd select the prope    | er methods for   | particular a   | pplic                             | ations.               |        |                   |  |
|  | • c  | reate Python code      | to implement a   | and apply th   | ese 1                             | methods to simple p   | oroble | ems               |  |
|  | • a  | pply the methods       | to organize and  | l manipulate   | e dat                             | a efficiently         |        |                   |  |
|  |  |                        |                  |                |                                   |                       |        |                   |  |
| 3  | Subject ai   | ms                     |                  |                |                                   |                       |        |                   |  |
|  | • [  | Data manipulation      | with Python      |                |                                   |                       |        |                   |  |
|  | • [  | Data visualization a   | nd reporting     |                |                                   |                       |        |                   |  |
|  | • S  | upervised learning     | g: regression ar | nd classificat | tion                              |                       |        |                   |  |
|  | • T  | Jnsupervised learn     | ing: clustering  | , dimension    | ality                             | reduction             |        |                   |  |
|  | Deep learning  |                        |                  |                |                                   |                       |        |                   |  |
|  | <ul> <li>Data storage and organization, databases of relevance in materials science</li> </ul> |                        |                  |                |                                   |                       |        |                   |  |
|  | • [  | Design and manage      | ement of datab   | ases           | 10.41                             |                       |        |                   |  |
| 4  | Teaching   | methods                |                  |                |                                   |                       |        |                   |  |
| -  | hands-on   | lectures and mini      | project          |                |                                   |                       |        |                   |  |
| 5  | Prerequis  | ites for participation | n                |                |                                   |                       |        |                   |  |
|  | Completie  | on of the modules      | "Programming     | g Concepts i   | n Ma                              | aterials Science" and | d "Ma  | aterials Infor-   |  |
|  | matics" is   | recommended            |                  |                |                                   |                       |        |                   |  |
| 6  | Assessme   | ent methods            |                  |                |                                   |                       |        |                   |  |
|  | Completio  | on of mini project     | with written pr  | oject report   |                                   |                       |        |                   |  |
| 7  | Prerequis  | ites for the assign    | nent of credit I | points         |                                   |                       |        |                   |  |
|  | Accepted   | project report         | -                |                |                                   |                       |        |                   |  |
| 8  | This mod   | ule is used in the f   | ollowing degre   | e programn     | nes a                             | s well                |        |                   |  |
|  | none   |                        | 0 0              |                |                                   |                       |        |                   |  |
| 9  | Impact or  | n total grade          |                  |                |                                   |                       |        |                   |  |
|  | 6/117  | C C                    |                  |                |                                   |                       |        |                   |  |
| 10                                       | Responsil  | bility for module      |                  |                |                                   |                       |        |                   |  |
|  | Prof. Dr. 1  | Drautz, Dr. Yury L     | ysogorskiy       |                |                                   |                       |        |                   |  |
| 11                                       | Other info   | ormation               |                  |                |                                   |                       |        |                   |  |
|  | Literature:  |                        |                  |                |                                   |                       |        |                   |  |
|  | Literature   | :                      |                  |                |                                   |                       |        |                   |  |
|  | W. McKir   | nney: Python for D     | ata Analysis: D  | ata Wrangli    | ng w                              | rith pandas, NumPy    | , and  | Jupyter, O'Reilly |  |
|  | (2022);  |                        |                  | 0              | 0                                 |                       |        |                   |  |
|  | J. Vander  | Plas: Python Data      | Science Handb    | ook: Essent    | ial T                             | ools for Working wi   | th Da  | ata, O'Reilly     |  |
|  | (2016);  | *                      |                  |                |                                   | 5                     |        | ,                 |  |
|  | J. Grus:Da   | ata Science from S     | cratch: First Pr | inciples wit   | les with Python, O'Reilly (2015). |                       |        |                   |  |

| INTRODUCTION TO PARALLEL- & SCIENTIFIC-COMPUTING |  |                        |  |                |              |                        |        |                    |  |
|--|--|------------------------|--|----------------|--------------|------------------------|--------|--------------------|--|
| Mod  | ule code   | Student                | Credits  | Semeste        | r            | Frequency              |        | Duration           |  |
|  | 7.3  | workload               | 6 ECTS   | 2nd            |              | summer term            |        | 1 semester         |  |
|  |  | 180 hours              |  |                |              |                        |        |                    |  |
| 1  | Types of o   | courses:               | Contact he   | ours           | Ind          | lependent study        | Clas   | ss size            |  |
|  | a) lectures  | 5                      | a) 30 hrs (2   | 2 SWS)         | 120          | ) hours                | 20 s   | students           |  |
|  | b) exercis   | es                     | b) 30 hrs (  | 2 SWS)         |              |                        |        |                    |  |
| 2  | Learning   | outcomes               |  |                |              |                        |        |                    |  |
|  | After suce   | cessful completion o   | f the module   | the students   | s hav        | ve gained knowledge    | e abo  | ut parallel pro-   |  |
|  | grammin  | g concepts. They car   | i translate a s  | erial algorith | ım i         | nto its parallel versi | on ar  | nd can apply par-  |  |
|  | allel conc   | epts to applications   | of scientific co   | omputing. T    | he s         | tudents have learne    | d and  | d applied the      |  |
|  | main imp   | ortant data commu      | nication conce   | epts in share  | ed m         | emory and distribut    | ted m  | nemory pro-        |  |
|  | grammin  | g via OpenMP and M     | API. The stud  | lents will ha  | ve ga        | ained practical prog   | ramn   | ning experience    |  |
|  | with specific problem oriented examples which support the experience in applying parallel compu-   |                        |  |                |              |                        |        |                    |  |
|  | ting methods. The students have worked on different numerical applications for which parallel algo-  |                        |  |                |              |                        |        |                    |  |
|  | nthins are introduced, compared and assessed. They have learned now to analyze the potential of a social program for its parallelization. The students will gain practical experience with numerical |                        |  |                |              |                        |        |                    |  |
|  | serial pro   | gram for its parallell | zation. The s  | ludents will   | gain<br>od b | i practical experienc  | e wit  | il numerical       |  |
|  | report   | ili computational pro  | Jects that wh  | ii be present  | eu D         | y the students in sir  | UIT LA | iiks allu a liilai |  |
| 3  | Subject a  | me                     |  |                |              |                        |        |                    |  |
| 5  | Parallel communication libraries MPI and OpenMP  |                        |  |                |              |                        |        |                    |  |
|  | <ul> <li>Parallel algorithms for particle methods, linear algebra</li> </ul>   |                        |  |                |              |                        |        |                    |  |
|  | • F  | erformance evaluat     | on   | unous, inica   | aig          | CDIa                   |        |                    |  |
|  | • 1  | Jumerical optimisat    | on   |                |              |                        |        |                    |  |
|  | • 4  | Application of nume    | rical libraries  |                |              |                        |        |                    |  |
| 4  | Teaching   | methods                | icui iibiuiico   |                |              |                        |        |                    |  |
| -  | lecture, cl  | ass-room exercises,    | project work   |                |              |                        |        |                    |  |
| 5  | Prerequis  | ites for participation |  |                |              |                        |        |                    |  |
|  | basic kno  | wledge in a higher p   | rogramming   | language       |              |                        |        |                    |  |
| 6  | Assessme   | ent methods            |  | 0 0            |              |                        |        |                    |  |
|  | project we   | ork on a given topic   | of scientific c  | omputing T     | rans         | lation of a problem    | into a | an OpenP or        |  |
|  | MPI versi  | on. Seminar talk an    | d written repo   | ort on the pr  | ojec         | t topic                |        |                    |  |
| 7  | Prerequis  | ites for the assignm   | ent of credit p  | points         |              |                        |        |                    |  |
|  | submissio  | on of report and pres  | sentation of p   | roject work    |              |                        |        |                    |  |
| 8  | This mod   | ule is used in the fo  | lowing degre   | e programn     | ies a        | is well                |        |                    |  |
|  | none   |                        |  |                |              |                        |        |                    |  |
| 9  | Impact of grade on total grade   |                        |  |                |              |                        |        |                    |  |
|  | 6/117  |                        |  |                |              |                        |        |                    |  |
| 10   | Responsi   | bility for module      |  |                |              |                        |        |                    |  |
|  | Prot. Dr.  | Godehard Sutmann       |  |                |              |                        |        |                    |  |
| 11   | Other inf  | ormation               | 1 .  | 4              |              | 1 • 1 • • •            |        | 1 C                |  |
|  | An online  | e repository provides  | es lecture notes (lecture files and video material), source code of pro- |                |              |                        |        |                    |  |
|  | grams discussed and developed during the class, and exercises with solutions.  |                        |  |                |              |                        |        |                    |  |



| PHYSICS OF COMPLEX PHASE TRANSITIONS IN SOLIDS |   |                         |                  |                 |                      |                       |       |                   |  |
|--|---|-------------------------|------------------|-----------------|----------------------|-----------------------|-------|-------------------|--|
| Mod  | ule code  | Student                 | Credits          | Semester        | ſ                    | Frequency             |       | Duration          |  |
|  | 7.4   | workload                | 6 ECTS           | 2nd             |                      | summer term           |       | 1 semester        |  |
|  |   | 180 hours               |                  |                 |                      |                       |       |                   |  |
| 1  | Types of o  | courses                 | Contact l        | hours           | Ind                  | lependent study       | Cla   | ss size           |  |
|  | a) lecture  |                         | a) 30 hrs        | (2 SWS)         | 120 hours20 students |                       |       |                   |  |
|  | b) semina   | ır                      | b) 30 hrs        | (2 SWS)         |                      |                       |       |                   |  |
| 2  | Learning  | outcomes                |                  |                 |                      |                       |       |                   |  |
|  | After part  | icipation in this m     | odule, studen    | its are able to | char                 | acterize and classify | 7 pha | se transitions in |  |
|  | solid state   | e materials. For the    | discussed ex     | amples (e.g. s  | supe                 | rconducting and fer   | roic  | phases) they      |  |
|  | know the  | underlying physica      | al concepts ar   | id scale-bridg  | ing 1                | methods to address    | these | 2.                |  |
|  | They are able to judge, compare and utilize these concepts and methods. |                         |                  |                 |                      |                       |       |                   |  |
| 3  | Subject aims  |                         |                  |                 |                      |                       |       |                   |  |
|  | • Introduction to complex phase transitions in solid state materials    |                         |                  |                 |                      |                       |       |                   |  |
|  | (e.g. magnetic, ferroelectric and superconducting phases)               |                         |                  |                 |                      |                       |       |                   |  |
|  | • Clas  | ssification of phase    | transitions a    | nd critical ph  | enor                 | nena                  |       |                   |  |
|  | (e.g  | order of phase tra      | nsitions, criti  | cal exponents   | s, ais               | placive transitions)  |       |                   |  |
|  | Models and simulation methods   |                         |                  |                 |                      |                       |       |                   |  |
|  | (e.g  | . spin models, Lan      | dau theory, m    | iolecular dyna  | amic                 | s simulations)        |       |                   |  |
| 4  | leaching  | methods                 |                  |                 |                      |                       |       |                   |  |
| 5  | Droroquio   | itaa far participatio   |                  |                 |                      |                       |       |                   |  |
| 2  | basic kno   | wledge on quantur       | n mechanica      | / solid state r | hvei                 | cs and thermodyna     | mice  | / statistical     |  |
|  | physics   | wieuge on quantui       | ii iiieciiaiiies | / solid state p | /11y51               | cs and mermouyna      | mes   |                   |  |
| 6  |   | ont methods             |                  |                 |                      |                       |       |                   |  |
| Ŭ  | Written a   | nd oral presentatio     | n of project w   | vork and shor   | t ora                | l examination relate  | ot be | project           |  |
| 7  | Prerequis   | ites for the assignment | nent of credit   | points          |                      |                       |       | F)                |  |
|  | taking pa   | rt in the seminar /     | project work     | 1               |                      |                       |       |                   |  |
| 8  | This mod  | ule is used in the f    | ollowing deg     | ree programn    | nes a                | s well                |       |                   |  |
|  | Physics   |                         | 0 0              | 1 0             |                      |                       |       |                   |  |
| 9  | Impact of   | grade on total grad     | de               |                 |                      |                       |       |                   |  |
|  | 6/117   |                         |                  |                 |                      |                       |       |                   |  |
| 10   | Responsi  | bility for module       |                  |                 |                      |                       |       |                   |  |
|  | Prof. Dr.   | Anna Grünebohm          | , Prof. Dr. Mi   | chael Scherer   | 1                    |                       |       |                   |  |
| 11   | Other inf   | ormation                |                  |                 |                      |                       |       |                   |  |
|  | Lecture notes will be provided.   |                         |                  |                 |                      |                       |       |                   |  |



| THE | THE CALPHAD METHOD IN THERMODYNAMICS AND DIFFUSION                                     |                        |       |                           |                |       |                        |         |                    |
|-----|--|------------------------|-------|---------------------------|----------------|-------|------------------------|---------|--------------------|
| Mod | ule code   | Student                |       | Credits                   | Semeste        | r     | Frequency              |         | Duration           |
|     | 7.5  | workload               |       | 6 ECTS                    | 2nd            |       | summer term            |         | 1 semester         |
|     |  | 180 hours              |       |                           |                |       |                        |         |                    |
| 1   | Types of o   | courses:               |       | Contact he                | ours           | Ind   | lependent study        | Cla     | ss size            |
|     | a) lecture   |                        |       | a) 45 hrs (               | 3 SWS)         | 120   | ) hours                | 15 s    | students           |
|     | b) class   |                        |       | b) 15 hrs (               | 1 SWS)         |       |                        |         |                    |
| 2   | Learning   | outcomes               |       |                           |                |       |                        |         |                    |
|     | Students   | understand the co      | nce   | pt of phase               | equilibrium    | , lea | rn how to model Gi     | bbs e   | energy and its de- |
|     | rivatives u  | using fundamental      | th    | eories and tl             | ne connectio   | n to  | experimental deter     | mine    | ed thermody-       |
|     | namic pro  | operties. They learn   | n to  | handle the                | rmodynami      | c and | d diffusion database   | s. Af   | ter a successful   |
|     | participat   | ion of the course s    | tud   | ents know t               | he mathema     | atica | l models of diffusio   | n ano   | d numerical        |
|     | methods  | as well as diffusion   | ı pı  | ocesses. Th               | ey will be ab  | le to | o understand physic    | al rel  | ationships in the  |
|     | diffusion  | process and the co     | nn    | ection to the             | e thermodyr    | ami   | c properties. They le  | earn    | to select a suita- |
|     | ble model  | according to a req     | lnii  | ement profi               | ile and are a  | ble t | o carry out simple r   | nater   | ial-specific simu- |
|     | lations of   | diffusion processe     | es in | n materials.              |                |       |                        |         |                    |
| 3   | Subject ai   | ms                     |       |                           |                |       |                        |         |                    |
|     | • 1  | hermodynamic fu        | nct   | ions and cal              | lculation of   | phas  | e diagrams.            |         |                    |
|     | Constructions of the CALPHAD-type computational thermodynamic databases after critical |                        |       |                           |                |       |                        |         |                    |
|     | evaluation of experimental information as well first- principles calculated data.      |                        |       |                           |                |       |                        |         |                    |
|     | <ul> <li>Microstructure simulations using thermodynamic quantities</li> </ul>          |                        |       |                           |                |       |                        |         |                    |
|     | • N  | Aathematical basic     | s o   | f the diffusion           | on equation    | diff  | fusivity, mobility coe | efficie | ents               |
|     | <ul> <li>Diffusion as a coupling of mobility and thermodynamics</li> </ul>             |                        |       |                           |                |       |                        |         |                    |
|     | Multicomponent Diffusion   |                        |       |                           |                |       |                        |         |                    |
|     | • I:   | ntroduction to DIC     | CTF   | RA                        |                |       |                        |         |                    |
|     | • N  | Aobility databases     |       |                           |                |       |                        |         |                    |
| 4   | Teaching   | methods                |       |                           |                |       |                        |         |                    |
|     | lecture, ex  | ercises, individual    | l pr  | oject, case s             | tudies, discu  | issic | ons, presentation of   | mod     | eling results      |
| 5   | Prerequis  | ites for participation | on    |                           |                |       |                        |         |                    |
|     | basic kno  | wledge in thermod      | lyn   | amics and s               | tatistical phy | vsics | , basic knowledge (    | of str  | ucture and prop-   |
|     | erties of n  | naterials, ordinary    | dif   | ferential equ             | lations.       |       |                        |         |                    |
| 6   | Assessme   | ent methods            |       |                           |                |       |                        |         |                    |
|     | written re   | port (10 to 15 page    | es) ( | of individua              | l project      |       |                        |         |                    |
| 7   | Prerequis  | ites for the assign    | me    | nt of credit <sub>I</sub> | points         |       |                        |         |                    |
|     | positively   | evaluated written      | rep   | ort                       |                |       |                        |         |                    |
| 8   | This mod   | ule is used in the f   | foll  | owing degre               | e programn     | ies a | is well                |         |                    |
|     | none   |                        |       |                           |                |       |                        |         |                    |
| 9   | Impact of  | grade on total gra     | de    |                           |                |       |                        |         |                    |
|     | 6/117  |                        |       |                           |                |       |                        |         |                    |
| 10  | Responsi   | bility for module      | _     |                           |                |       |                        |         |                    |
|     | Prot. Dr.  | Ingo Steinbach, Di     | r. Jı | ulia Kundin               |                |       |                        |         |                    |
| 11  | Other info   | ormation               |       |                           |                |       |                        |         |                    |
|     | Literature   |                        |       |                           |                |       | 1                      |         | .1 1 7             |
|     | H.L. Luka  | is, S.G. Fries, B. Si  | inc   | Iman: Comp                | outational th  | erm   | odynamics, the Cal     | phad    | method, Cam-       |
|     | bridge Ur  | iversity Press (200    | )/).  |                           | -1.1.171       | 1     |                        | 1.1     |                    |
|     | A. Paul, I   | . Laurila, V. Vuori    | ner   | 1, S.V. Divin             | iski: Thermo   | odyn  | amics, Diffusion an    | d the   | e Kirkendall Ef-   |
|     | fect in Solids, Springer, Cham, (2014).  |                        |       |                           |                |       |                        |         |                    |



| FUNDAMENTAL ASPECTS OF MATERIALS SCIENCE AND ENGINEERING |  |                         |                   |                |         |                       |        |                   |  |
|--|--|-------------------------|-------------------|----------------|---------|-----------------------|--------|-------------------|--|
| (FAN   | ISE)   |                         |                   |                |         |                       |        |                   |  |
| Mod  | ule code   | Student                 | Credits           | Semeste        | er      | Frequency             |        | Duration          |  |
|  | 7.6  | workload                | 6 ECTS            | 2nd            |         | summer term           |        | 1 semester        |  |
|  |  | 180 hours               |                   |                |         |                       |        |                   |  |
| 1  | Types of o   | courses:                | Contact ho        | ours           | Ind     | ependent study        | Cla    | ss size           |  |
|  | a) lecture   |                         | a) 45 hrs (3      | 3 SWS)         | 120     | hours                 | a) 1   | 10 students       |  |
|  | b) class   |                         | b) 15 hrs (       | 1 SWS)         |         |                       | b) 1   | 0 students        |  |
| 2  | Learning   | outcomes                |                   |                |         |                       |        |                   |  |
|  | Students   | will be able to appl    | y elements from   | m the mater    | rials s | science curriculum    | to ac  | tual engineering  |  |
|  | problems   | in advanced mater       | rials technology  | 7. They are a  | ware    | of the strong link l  | betwo  | een elementary    |  |
|  | atomistic,   | crystallographic, t     | hermodynamic      | c/kinetic and  | d mic   | crostructural proces  | ses a  | nd the behav-     |  |
|  | iour of m  | aterials/componen       | ts on the macro   | o scale. The   | y will  | be able to use the    | unde   | rstanding of      |  |
|  | basic proc   | cesses to develop n     | ew and improv     | e classical n  | nateri  | ials, to assess the m | iecha  | inical and func-  |  |
|  | tional pro   | perties of material     | s and to unders   | stand kinetio  | c proo  | cesses in solids and  | l at s | urfaces. In addi- |  |
|  | tion to an   | increased familiar      | ity with advanc   | ed basic cor   | ncept   | s, the students will  | be al  | ble to apply ma-  |  |
|  | terials sci  | ence theory to four     | fascinating ma    | aterial classe | es: H   | igh entropy alloys,   | inter  | metallic phases,  |  |
| -  | single crystal NI-base superalloys and snape memory alloys.                                  |                         |                   |                |         |                       |        |                   |  |
| 3  | Subject an   | ms                      | 1 1 .             |                |         | 1.1 .                 |        |                   |  |
|  | • 1:   | mportance of atom       | is and electrons  | s in materia.  | ls eng  | gineering and the t   | ransı  | tion from atoms   |  |
|  | te   | o alloys and from a     | lloys to compo    | nents          |         | 10 1 1                | c      | 11 1 • / •.1      |  |
|  | • 1  | nermodynamic co         | ncepts in mate    | rials engine   | ering   | g and fundamentals    | s of a | lloy design (with |  |
|  | a  | special focus on te     | ernary phase di   | agrams)        |         | • / • 11              |        | . ,               |  |
|  | • Kinetic concepts in materials science and engineering (especially precipitation processes) |                         |                   |                |         |                       |        |                   |  |
|  |  | asic concepts of so     | nia state phase   | transforma     | tions   |                       | . 1    |                   |  |
|  | • (  | nderstanding and        | application of    | knowledge      | to 101  | ar materials classes  | : n1g  | n entropy alloys, |  |
|  | 11   | ntermetanic phases      | s, single crystal | superanoys     | ana     | snape memory and      | oys    | mallarra)         |  |
|  | • <i>P</i>   | cquisition of know      | ledge about fin   | gn tempera     | ture s  | strengtn (example:    | supe   | ralloys)          |  |
| 4  | Teaching   | methods                 | ledge about frac  | lure mechar    | lics a  | nd laugue (example    | . sna  | be memory alloys) |  |
| 4  | lecture cl   | neurous                 |                   |                |         |                       |        |                   |  |
| 5  | Prerequis  | ites for participatic   | m                 |                |         |                       |        |                   |  |
| <b>,</b>   | successfu  | l completion of "Fl     | ements of Mic     | rostructure"   | ' (2a)  | and "Statistical Me   | char   | uics and Funda-   |  |
|  | mental M   | aterials Physics" (2    | c) recommend      | led            | (24)    | und Statistical me    | ciiui  | iles ulla i ullau |  |
| 6  | Assessme   | ent methods             |                   |                |         |                       |        |                   |  |
|  | oral exam  | ination (0.5 hours)     |                   |                |         |                       |        |                   |  |
| 7  | Prerequis  | ites for the assignment | nent of credit r  | ooints         |         |                       |        |                   |  |
|  | passing th   | ne exam                 | <b>- -</b>        |                |         |                       |        |                   |  |
| 8  | This mod   | ule is used in the f    | ollowing degre    | e programn     | nes as  | s well                |        |                   |  |
|  | Master of Science in Mechanical Engineering: Werkstoff- und Microengineering                 |                         |                   |                |         |                       |        |                   |  |
| 9  | Impact of  | grade on total grad     | de                | 0              |         |                       |        |                   |  |
|  | 6/117  | - 0                     |                   |                |         |                       |        |                   |  |
| 10   | Responsi   | bility for module       |                   |                |         |                       |        |                   |  |
|  | Prof. Dr   | Ing. Gunther Egge       | ler               |                |         |                       |        |                   |  |
| 11   | Other info   | ormation                |                   |                |         |                       |        |                   |  |
|  | A list with recommended literature and class notes will be available online.                 |                         |                   |                |         |                       |        |                   |  |



| POLYMERS AND SHAPE MEMORY ALLOYS |   |                          |                  |               |        |                      |        |                    |  |
|----------------------------------|---|--------------------------|------------------|---------------|--------|----------------------|--------|--------------------|--|
| Mod                              | lule code   | Student                  | Credits          | Semeste       | r      | Frequency            |        | Duration           |  |
|                                  | 7.7   | workload                 | 6 ECTS           | 2nd           |        | summer term          |        | 1 semester         |  |
|                                  |   | 180 hours                |                  |               |        |                      |        |                    |  |
| 1                                | Types of o  | courses:                 | Contact ho       | ours          | Ind    | lependent study      | Cla    | ss size            |  |
|                                  | a) lecture  |                          | a) 45 hrs (3     | (3 SWS) 120   |        | ) hours              | a) 1   | 0 students         |  |
|                                  | b) class  |                          | b) 15 hrs (      | 1 SWS)        |        |                      | b) 1   | 10 students        |  |
| 2                                | Learning  | outcomes                 |                  |               |        |                      |        |                    |  |
|                                  | Students  | will be familiar wit     | h the morphol    | ogy/microst   | ructi  | ure of polymers and  | l sha  | pe memory al-      |  |
|                                  | loys and l  | cnow how to proces       | ss these materi  | als. They wi  | ll un  | derstand the basic r | mech   | anical and func-   |  |
|                                  | tional pro  | perties of these two     | o materials clas | sses with a s | pecia  | al focus on enginee  | ring   | applications and   |  |
|                                  | be familia  | ar with scale bridgi     | ng concepts, i.e | e. they can d | 1SCUS  | ss macroscopic prop  | pertie | es in view of at-  |  |
|                                  | omistic ir  | iteractions and mo       | rphological/mi   | crostructura  | li tea | itures. Most importa | antiy  | , they will under- |  |
| 2                                | Stand the   | relation between n       | norphology/mi    | crostructure  | and    | i mechanical and fu  | nctic  | mai properties.    |  |
| 5                                |   | uns<br>Processing and mo | mbology of pol   | umore         |        |                      |        |                    |  |
|                                  |   | Therestorization of      | polymore         | ymers         |        |                      |        |                    |  |
|                                  |   | hysical and therm        | polymers         | cts of polym  | or m   | nterials science     |        |                    |  |
|                                  | <ul> <li>Mechanical and functional properties of polymers and engineering applications</li> </ul> |                          |                  |               |        |                      |        |                    |  |
|                                  | • 1   | ntroduction of the       | shape memory     | effects in c  | weta   | lline materials      | prica  | 10115              |  |
|                                  | • 1   | Thereacterization of     | shape memory     | allovs        | ysta   |                      |        |                    |  |
|                                  | • •   | ole of the martens       | itic transforma  | tion in shar  | e m    | emory technology     |        |                    |  |
|                                  | • 1   | Aechanical and fur       | ictional propert | ties of shape | me     | mory alloys          |        |                    |  |
| 4                                | Teaching  | methods                  |                  | r -           |        |                      |        |                    |  |
|                                  | lecture, cl   | ass                      |                  |               |        |                      |        |                    |  |
| 5                                | Prerequis   | ites for participation   | n                |               |        |                      |        |                    |  |
|                                  | successfu   | l completion of "El      | ements of Mic    | rostructure"  | (2a)   | or equivalent recor  | nme    | nded               |  |
| 6                                | Assessme  | ent methods              |                  |               |        |                      |        |                    |  |
|                                  | written ex  | amination (2 hour        | s)               |               |        |                      |        |                    |  |
| 7                                | Prerequis   | ites for the assignr     | nent of credit p | points        |        |                      |        |                    |  |
|                                  | passing th  | ne written examina       | tion             |               |        |                      |        |                    |  |
| 8                                | This mod  | ule is used in the f     | ollowing degre   | e programn    | ies a  | s well               |        |                    |  |
|                                  | Master of   | Science in Mechai        | nical Engineeri  | ng: Werksto   | ff-E1  | ngineering           |        |                    |  |
| 9                                | Impact of   | grade on total grad      | de               |               |        |                      |        |                    |  |
|                                  | 6/117   |                          |                  |               |        |                      |        |                    |  |
| 10                               | Responsi  | Dility for module        | Ing Ice From     |               |        |                      |        |                    |  |
| 11                               | Dr. Kiaus   | Neuking, Prof. Dr        | ing. Jan Fren    | zei           |        |                      |        |                    |  |
| 11                               | Lecture n   | otes will be provide     | d                |               |        |                      |        |                    |  |
|                                  | Lecture notes will be provided.   |                          |                  |               |        |                      |        |                    |  |



| COM | COMPUTATIONAL PLASTICITY |                            |                 |                  |        |                           |                  |                                       |  |  |
|-----|--------------------------|----------------------------|-----------------|------------------|--------|---------------------------|------------------|---------------------------------------|--|--|
| Mod | ule code                 | Student                    | Credits         | Semester         |        | Frequency                 |                  | Duration                              |  |  |
|     | 7.8                      | workload                   | 6 ECTS          | 2nd              |        | summer term               |                  | 1 semester                            |  |  |
|     |                          | 180 hours                  |                 |                  |        |                           |                  |                                       |  |  |
| 1   | Types of o               | courses                    | Contact l       | nours            | Ind    | lependent study           | Clas             | ss size                               |  |  |
|     | lecture an               | id class                   | 60 hrs (4       | SWS)             | 120    | ) hours                   | no i             | restrictions                          |  |  |
| 2   | Learning                 | outcomes                   |                 | مرور مرور مرور   |        | ماليالية بالمكرية بالمراد | c 1:00           | and the second                        |  |  |
|     | After succ               | essiully completing        | g the module    | , the students   | fied   | They understand t         | l allie<br>ho nh | erent types of                        |  |  |
|     | and mech                 | anisms of elastic a        | nd plastic bel  | avior of cryst   | allir  | e materials and car       | no pi<br>nontl   | ine the different                     |  |  |
|     | types of p               | lasticity models in        | solid mechan    | ics. Furtherm    | lore   | , they can explain th     | e bas            | sic concepts and                      |  |  |
|     | the mathe                | ematical formulation       | on of continu   | um plasticity a  | and    | crystal plasticity. Th    | ey di            | scuss the basic                       |  |  |
|     | concepts                 | of the numerical in        | nplementatio    | n of plasticity  | mo     | dels and identify the     | e met            | hod which is                          |  |  |
|     | most suit                | ed to solve a given        | mechanical p    | roblem. Stude    | ents   | can implement and         | l app            | ly a numerical                        |  |  |
|     | scheme fo                | or the solution of e       | lasto-plastic p | roblems with     | in th  | ne finite element me      | ethod            | •                                     |  |  |
| 3   | Subject ai               | ms                         | 1.              | 1                |        | 1 .                       |                  |                                       |  |  |
|     |                          | Sasics of continuum        | n mechanics     | and Finite Ele   | mer    | nt Analysis               |                  |                                       |  |  |
|     | • •                      | nenomenology an            | d atomistic of  | uiold critori    | anc    | l plastic deformation     | n<br>nd bi       | nomatic hardon                        |  |  |
|     | • (                      | 2011Cepts of Continu       | ium plasticity  | (yield chiello   | )11, 1 | iow rule, isotropic a     | nu ki            | inematic naruen-                      |  |  |
|     | • •                      | 118)<br>Rate dependent and | l rate-indepen  | dent formula     | tion   | s of continuum play       | sticity          | 7                                     |  |  |
|     | • 1                      | Sumerical solution         | schemes for     | elasto-plastici  | tv (o  | perator split, return     | mar              | pping, consistent                     |  |  |
|     | ta                       | angent modulus)            |                 | F                | -) (-  | F                         | r                | · · · · · · · · · · · · · · · · · · · |  |  |
|     | • (                      | Computational aspe         | ects of small a | ind large strai  | n fo   | rmulations                |                  |                                       |  |  |
|     | • (                      | Concepts of crystal        | plasticity (dis | location slip, i | low    | rule, hardening mo        | dels,            | consistent tan-                       |  |  |
|     | g                        | ent modulus)               |                 |                  |        |                           |                  |                                       |  |  |
|     | • \$                     | structure, impleme         | ntation and a   | pplication of a  | an A   | baqus UMAT                |                  |                                       |  |  |
| 4   | Teaching                 | methods                    |                 |                  | 1      |                           |                  |                                       |  |  |
| F   | lecture, h               | ands-on classes, m         | ini project ind | cl. seminar tal  | k, as  | ssignments                |                  |                                       |  |  |
| 5   | none                     | nes for participatio       | 011             |                  |        |                           |                  |                                       |  |  |
| 6   | Assessme                 | ent methods                |                 |                  |        |                           |                  |                                       |  |  |
|     | Portfolio                | exam including rep         | orts on assig   | nments, semi     | nar    | and self-evaluation       | repoi            | rt                                    |  |  |
| 7   | Prerequis                | ites for the assignr       | nent of credit  | points           |        |                           |                  |                                       |  |  |
|     | passed fir               | nal module examin          | ation           |                  |        |                           |                  |                                       |  |  |
| 8   | This mod                 | ule is used in the f       | ollowing deg    | ree programm     | ies a  | is well                   |                  |                                       |  |  |
|     | Master of                | Science Computat           | tional Engine   | ering, Master    | of S   | cience Maschinenb         | au               |                                       |  |  |
| 9   | Impact of                | grade on total grad        | de              |                  |        |                           |                  |                                       |  |  |
| 10  | 0/11/<br>Bognon-:1       | hility for modul-          |                 |                  |        |                           |                  |                                       |  |  |
| 10  | Prof Dr                  | Alexander Hartma           | ier             |                  |        |                           |                  |                                       |  |  |
| 11  | Other inf                | ormation                   | 101             |                  |        |                           |                  |                                       |  |  |
|     | Lecture n                | otes will be provide       | ed.             |                  |        |                           |                  |                                       |  |  |



| ENGINEERING CERAMICS & COATING TECHNOLOGY |            |                      |                        |                          |   |                      |        |                    |  |
|---|------------|----------------------|------------------------|--------------------------|---|----------------------|--------|--------------------|--|
| Mod                                       | ule code   | Student              | Credits                | Semeste                  | er                                      | Frequency            |        | Duration           |  |
|   | 7.9        | workload             | 6 ECTS                 | 2nd                      |   | summer term          |        | 1 semester         |  |
|   |            | 180 hours            |                        |                          |   |                      |        |                    |  |
| 1   | Types of o | courses:             | Contact he             | ours                     | Ind                                     | lependent study      | Cla    | ss size            |  |
|   | a) lecture |                      | a) 30 hrs (            | 2 SWS)                   | 135                                     | 5 hours a)           |        | a) 10 students     |  |
|   | b) class   |                      | b) 30 hrs (            | 2 SWS)                   |   |                      | b) 1   | 10 students        |  |
| 2   | Learning   | outcomes             |                        |                          |   |                      |        |                    |  |
|   | The stude  | ents obtain a profo  | und knowledge          | of engineer              | ring                                    | ceramics and their t | techr  | ical applications. |  |
|   | By examp   | les, they learn and  | understand th          | e major pro              | cessi                                   | ing steps in manufa  | cturi  | ng engineering     |  |
|   | ceramics   | and in manufactur    | ring routes for        | fibre-reinfor            | ced                                     | ceramic matrix com   | iposi  | tes. They become   |  |
|   | familiar w | vith the typical the | rmo-mechanica          | l and functi             | ional                                   | properties of ceran  | nics.  | This knowledge     |  |
|   | enables th | ne students to selec | ct ceramics for        | specific nee             | ds.                                     |                      |        |                    |  |
|   | In additio | n, the students gai  | in basic knowle        | dge on coat              | ing t                                   | echnologies for thic | k lay  | ers of ceramic     |  |
|   | materials, | , including therma   | l spray and sin        | tering techn             | olog                                    | ies, which enables t | he st  | udents to select   |  |
|   | suitable c | oating methods for   | r wear, corrosic       | on, function             | al an                                   | d high temperature   | appl   | ications.          |  |
| 3   | Subject ai | ms                   | 1                      |                          |   | c .                  |        |                    |  |
|   | • P        | owder synthesis &    | conditioning,          | shaping, sir             | iterii                                  | ng of ceramic mater  | ials   |                    |  |
|   | • (        | characterisation of  | ceramics with          | different me             | etho                                    | ds                   |        |                    |  |
|   | • P        | Properties and appl  | lications of eng       | ineering cer             | ami                                     | cs                   |        |                    |  |
|   | • E        | Basic knowledge or   | different thick        | t film depos             | ition                                   | technologies (them   | nal s  | pray processes     |  |
|   | а          | nd sintering techn   | iques)                 |                          |   |                      |        |                    |  |
|   | • [        | Demonstration how    | v coatings can i       | mprove the               | func                                    | ctionality of compor | nents  |                    |  |
| 4   | Teaching   | methods              |                        |                          |   |                      |        |                    |  |
| 5   | Proroquia  | itog for participati | ~~~                    |                          |   |                      |        |                    |  |
| 2   | knowledg   | e in materials pror  | n<br>Derties is recorr | mended                   |   |                      |        |                    |  |
| 6   | Assessme   | ent methods          | Jerties is recom       | inicilaca.               |   |                      |        |                    |  |
| Ŭ   | written re | port on assignmer    | nt (weight for fi      | nal grade <sup>.</sup> 3 | 0%)·                                    |                      |        |                    |  |
|   | oral exam  | ination (20 minute   | es) or written e       | ramination               | (90 r                                   | ninutes) (weight for | fina   | l grade: 70%)      |  |
| 7   | Prerequis  | ites for the assign  | ment of credit i       | oints                    | (,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |                      |        | i gradot / d / d / |  |
|   | passing th | ne exam              |                        |                          |   |                      |        |                    |  |
| 8   | This mod   | ule is used in the f | following degre        | e programn               | nes a                                   | is well              |        |                    |  |
|   | Master of  | Science in Mecha     | nical Engineeri        | ng: Werksto              | off-E                                   | ngineering           |        |                    |  |
| 9   | Impact of  | grade on total gra   | de                     |                          |   |                      |        |                    |  |
|   | 6/117      |                      |                        |                          |   |                      |        |                    |  |
| 10  | Responsi   | bility for module    |                        |                          |   |                      |        |                    |  |
|   | Prof. Dr.  | Robert Vaßen         |                        |                          |   |                      |        |                    |  |
| 11  | Other info | ormation             |                        |                          |   |                      |        |                    |  |
|   | Literature | :                    | <b>.</b>               |                          |   |                      |        |                    |  |
|   | Ceramic l  | Materials, Science   | and Engineerir         | ıg, C. Barry             | Cart                                    | er, M. Grant Nortor  | ı, Spi | ringer 2013;       |  |
|   | Handboo    | k of Properties of   | l'echnical & En        | gineering C              | eran                                    | nics, R. Morrell, HM | ISO :  | 1989;              |  |
|   | Ceramics   | , D. Munz, T. Fett,  | Springer, 1999         | );<br>1. · 1             | 1 ~                                     |                      |        | 7 TT . 1 .         |  |
|   | The Mech   | anics and Reliabil   | ity of Films, M        | ultilayers an            | d Co                                    | oatings, M.R. Begley | 7, J.W | . Hutchinson,      |  |
|   | Cambridg   | ge University Press  | s, 2017;               | w/:1 2000                |   |                      |        |                    |  |
|   | Plasma S   | pray Coating, Robe   | ert B. Heiman,         | wiley, 2008              | •                                       |                      |        |                    |  |
|   | Slides wil | i de available onlin | ie.                    |                          |   |                      |        |                    |  |



| THE | ORY OF      | ELECTRONIC                | EXCITATI        | ONS IN M                           | <b>\TE</b> | RIALS                  |         |                   |
|-----|-------------|---------------------------|-----------------|------------------------------------|------------|------------------------|---------|-------------------|
| Mod | ule code    | Student                   | Credits         | Semester                           |            | Frequency              |         | Duration          |
|     | 7.10        | workload                  | 6 ECTS          | 2nd                                |            | summer term            |         | 1 semester        |
|     |             | 180 hours                 |                 |                                    |            |                        |         |                   |
| 1   | Types of o  | courses                   | Contact         | hours                              | Ind        | lependent study        | Cla     | ss size           |
|     | a) lecture  |                           | a) 30 hrs       | (2 SWS                             | 120        | ) hours                | 20 s    | students          |
|     | b) hands-   | on                        | b) 30 hrs       | ; (2 SWS)                          |            |                        |         |                   |
| 2   | Learning    | outcomes                  | _               |                                    |            |                        |         |                   |
|     | Electronic  | c Structure Theory        | is a successfu  | ıl and growin                      | g are      | ea of materials scien  | ce, ta  | aking advantage   |
|     | of the inc  | reasing availability      | of high perfo   | ormance com                        | outer      | rs. Starting only from | n the   | e knowledge of    |
|     | the types   | of atoms that make        | e up the syste  | m (molecule,                       | crys       | tal, nanostructure, .  | ), st   | udents will learn |
|     | how to ac   | curately calculate t      | he response j   | properties of r                    | nate       | rials without any fu   | rther   | experimental      |
|     | input, i.e. | using only the fur        | idamental lav   | vs of electrody                    | man        | nics and quantum p     | hysic   | s. Students get   |
|     | familiar w  | vith state-of-the-art     | theoretical a   | nd computation                     | onal       | approaches to elect    | conic   | excitations and   |
|     | theoretica  | a spectroscopy (dei       | Isity function  | lai theory, tim                    | e-ae       | pendent density fur    | 1CT101  | hal theory,       |
|     | Green's n   | unction methods).         | In practical c  | lasses, studer                     | ts ga      | ain nands-on experi    | ence    | in the use of     |
|     | various so  | onware packages ic        | of electronic s | aructure sinit                     |            | they leave here to co  | na si   | ate. In the final |
|     | and analy   | ey undertake a sind       | numerical re    | i project ili wi                   | IICII      | they learn now to ca   | III y O | out simulations   |
| 3   | Subject a   | ime                       | inumericarie    | suits.                             |            |                        |         |                   |
| 5   | Four        | indations of theory       | for interactir  | ng electrons. r                    | near       | fields and auviliars   | evet    | ems narticles     |
|     | and         | auasinarticles fur        | ictionals in m  | ig ciccuoiis. I<br>ianv-narticle i | hvsi       | ics                    | syst    | cills, particies  |
|     | • Flee      | tronic excitations        | narticle-hole   | excitations co                     | ollect     | tive excitations exci  | tatio   | ns in 2D 1D 0D    |
|     | nan         | ostructures               | purticie noie   | exertations, et                    | ince       | uve excitations, exci  | uuioi   | 15 III 2D, 1D, 0D |
|     | • Line      | ear response and e        | xcitation ener  | rgies                              |            |                        |         |                   |
|     | • Moo       | deling neutral excit      | ations by tim   | e-dependent                        | dens       | sity functional theor  | v       |                   |
|     | • Moo       | deling charged and        | neutral excit   | ations by Gre                      | en's       | function methods       | /       |                   |
|     | • App       | olications to spectro     | oscopy          |                                    |            |                        |         |                   |
| 4   | Teaching    | methods                   | 17              |                                    |            |                        |         |                   |
|     | Lectures,   | hands-on compute          | er classes, ind | ividual projec                     | t          |                        |         |                   |
| 5   | Prerequis   | ites for participation    | on              | <b>*</b> '                         |            |                        |         |                   |
|     | Knowledg    | ge of linux/unix en       | vironment, co   | ompletion of '                     | Fun        | damental Materials     | Phys    | ics" or           |
|     | equivalen   | t courses is recom        | mended          |                                    |            |                        |         |                   |
| 6   | Assessme    | ent methods               |                 |                                    |            |                        |         |                   |
|     | Oral exan   | nination (0.5 h) on       | the content o   | f the lecture,                     | inclu      | uding a short preser   | tatio   | n (<10 minutes)   |
|     | on the con  | mputational projec        | t. Bonus poir   | its can be gaii                    | ied l      | by presenting solution | ons te  | o the worksheets  |
|     | in class.   |                           |                 |                                    |            |                        |         |                   |
| 7   | Prerequis   | ites for the assign       | nent of credi   | t points                           |            |                        |         |                   |
|     | Passing th  | he oral examination       | n               |                                    |            | 11                     |         |                   |
| 8   | This mod    | ule is used in the f      | ollowing deg    | ree programn                       | ies a      | is well                |         |                   |
| 0   | Physics     |                           | 4.              |                                    |            |                        |         |                   |
| 9   |             | grade on total gra        | ae              |                                    |            |                        |         |                   |
| 10  | 0/11/       | hility for modulo         |                 |                                    |            |                        |         |                   |
| 10  | Prof Dr     | Silvana Botti             |                 |                                    |            |                        |         |                   |
| 11  | Other inf   | ormation                  |                 |                                    |            |                        |         |                   |
| 11  | Recomme     | ended literature R        | ichard M Ma     | rtin "Flectro                      | nic S      | tructure" Cambrida     | e Un    | iversity Press    |
|     | Richard N   | $\Lambda$ Martin Lucia Re | ining David     | M Cenerlev                         | "Int       | eracting Electrons"    | Cam     | ibridge           |
|     | Universit   | v Press.                  |                 | in cepency,                        | 1110       | eracung Licenoils      | Jaill   | 1011460           |
|     |             | /                         |                 |                                    |            |                        |         |                   |

| PHASE-FIELD THEURY AND APPLICATION   |   |  |  |  |  |  |  |  |
|--|---|--|--|--|--|--|--|--|
| Module code Student Credits Semester Frequency   | Duration  |  |  |  |  |  |  |  |
| 7.11 workload 6 ECTS 2nd winter term   | 1 semester  |  |  |  |  |  |  |  |
| 180 hours  |   |  |  |  |  |  |  |  |
| 1         Types of courses:         Contact hours         Independent study                      | Class size  |  |  |  |  |  |  |  |
| a) lecture a) 45 hrs (3 SWS) 120 hours   | a) 30 students  |  |  |  |  |  |  |  |
| b) exercises b) 15 hrs (1 SWS)   | b) 10-15 students   |  |  |  |  |  |  |  |
| 2 Learning outcomes  |   |  |  |  |  |  |  |  |
| The students understand the principles of mesoscopic structure formation in o                    | condensed matter as   |  |  |  |  |  |  |  |
| the basis of the phase-field theory. They are able to derive the basic relations of              | t this theory and relate  |  |  |  |  |  |  |  |
| the parameters to measurable physical quantities. They are able to use theoret                   | ical methods to inves-  |  |  |  |  |  |  |  |
| tigate scale separation in condensed matter. The students are skilled in the app                 | tigate scale separation in condensed matter. The students are skilled in the application of the phase-<br>field theory in numerical simulations. In the practical exercises, they developed a simple software |  |  |  |  |  |  |  |
| field theory in numerical simulations. In the practical exercises, they develope                 | field theory in numerical simulations. In the practical exercises, they developed a simple software   |  |  |  |  |  |  |  |
| code to simulate dendritic growth in 3D, thus being able to independently formulate new branches |   |  |  |  |  |  |  |  |
| of the simulation software developed at ICAMS.   |   |  |  |  |  |  |  |  |
| 5 Subject anns<br>Dendric solidification, scale invariant solution and microscopic solvability   |   |  |  |  |  |  |  |  |
| Traveling wave solution of a phase front sharp and thin interface limit                          |   |  |  |  |  |  |  |  |
| Anisotropy and the E-vector approach   |   |  |  |  |  |  |  |  |
| Coupling to outer fields, elasticity   |   |  |  |  |  |  |  |  |
| Coupling to multiphase flow via the Lattice Boltzmann method                                     |   |  |  |  |  |  |  |  |
| Microscopic variables and fluctuations, extension to critical phenomena                          |   |  |  |  |  |  |  |  |
| Miscellaneous applications in materials science  |   |  |  |  |  |  |  |  |
| 4 Teaching methods   |   |  |  |  |  |  |  |  |
| lecture, exercises   |   |  |  |  |  |  |  |  |
| 5 Prerequisites for participation  |   |  |  |  |  |  |  |  |
| Students must have good knowledge in statistical and condensed matter physi                      | cs. Programming   |  |  |  |  |  |  |  |
| skills in C++ are of advantage.  |   |  |  |  |  |  |  |  |
| 6 Assessment methods   |   |  |  |  |  |  |  |  |
| written exam (2 hours)   |   |  |  |  |  |  |  |  |
| 7 Prerequisites for the assignment of credit points  |   |  |  |  |  |  |  |  |
| passing the written examination  |   |  |  |  |  |  |  |  |
| 8 This module is used in the following degree programmes as well                                 |   |  |  |  |  |  |  |  |
| 10000 Impact of grade on total grade   |   |  |  |  |  |  |  |  |
| 6 /117   |   |  |  |  |  |  |  |  |
| 10 Responsibility for module   |   |  |  |  |  |  |  |  |
| Prof Dr Ingo Steinbach Prof Dr Fathollah Varnik Dr Oleg Shchyglo                                 |   |  |  |  |  |  |  |  |
| 11 Other information   |   |  |  |  |  |  |  |  |
| Lecture notes will be provided online.   |   |  |  |  |  |  |  |  |

| MUL | .TISCALI    | E MECHANICS             | OF MATE             | RIALS           |        |                        |         |                   |
|-----|-------------|-------------------------|---------------------|-----------------|--------|------------------------|---------|-------------------|
| Mod | ule code    | Student                 | Credits             | Semester        | ſ      | Frequency              |         | Duration          |
|     | 7.12        | workload                | 6 ECTS              | 3rd             |        | winter term            |         | 1 semester        |
|     |             | 180 hours               |                     |                 | _      |                        |         |                   |
| 1   | Types of o  | courses                 | Contact I           | hours           | Inc    | lependent study        | Clas    | s size            |
|     | a) lecture  |                         | a) $30 \text{ hrs}$ | (2 SWS)         | 120    | ) hours                | a) 20   | 0 students        |
| 2   | D) Class    |                         | D) 30 hrs           | (2 SWS)         |        |                        | D) 10   | 0 students        |
| 2   | Learning    | outcomes                | ltiggalo patur      | o of the most   | oni    | cal behaviour of ma    | toriala | and of the dif    |
|     | foront apr  | aroachag to take thi    | g into accoun       | t in mochani    | col n  | nodelling of micros    | tructu  | rog Thoy can      |
|     | idontify th | no relevant length      | s into account      | n in mechanic   |        | nouening of finitios   | .Tuctu  | moso /macro       |
|     | scopic str  | ic icievant iciigin-    | ationshing T        | he students u   | ndei   | rstand the principle   | s of ef | fective theory    |
|     | construct   | ion coarse graining     | and homog           | enisation met   | thod   | s and they can appl    | v ther  | n to identify     |
|     | analyse at  | nd model multiscal      | e problems          | such as plastic | c def  | Formation hardenin     | o heh   | aviour and frac-  |
|     | ture of m   | icrostructures. The     | v are able to 1     | use state of th | e art  | numerical and the      | oretic  | al scale-bridging |
|     | modelling   | g methods. They ca      | n apply num         | erical tools or | ı diff | ferent length scales.  | and ı   | understand the    |
|     | underlyin   | g principles (atomi     | stic modellin       | g, discrete di  | sloca  | ation dynamics, con    | tinuu   | m plasticity).    |
| 3   | Subject a   | ims                     |                     | 0               |        | •                      |         | * */              |
|     | • S         | State of the art in br  | idging lengtł       | n-scales in mo  | odeli  | ng of elasticity, plas | ticity, | and fracture      |
|     | • F         | Principles and conc     | epts of concu       | rrent and hie   | rarcl  | hical multiscale mo    | deling  | g of materials    |
|     | • E         | Basics of atomistic 1   | nodeling: fro       | m density fu    | nctio  | onal theory to large s | scale r | nolecular dy-     |
|     | r           | namics                  | 0                   | ·               |        |                        |         |                   |
|     | • [         | Defect identification   | ı in atomistic      | simulations     |        |                        |         |                   |
|     | • [         | Discrete dislocation    | dynamics            |                 |        |                        |         |                   |
|     | • (         | Crystal plasticity: ph  | ienomenolog         | ical and dens   | ity b  | ased methods           |         |                   |
|     | • H         | Homogenization m        | ethods              |                 |        |                        |         |                   |
| 4   | Teaching    | methods                 |                     |                 |        |                        |         |                   |
|     | lecture, co | omputer exercises,      | and seminar         |                 |        |                        |         |                   |
| 5   | Prerequis   | ites for participatio   | n                   |                 |        |                        |         |                   |
|     | successfu   | l completion of "Ba     | asics in Mater      | rials Science"  | (mo    | odule 2) or equivaler  | ıt      |                   |
| 6   | Assessme    | ent methods             | <b>.</b> .          |                 |        |                        |         |                   |
|     | oral (0.5 h | nours) or written (2    | hours) exam         | ination, depe   | ndin   | ig on size of the clas | S       |                   |
| 7   | Prerequis   | ites for the assignment | nent of credit      | points          |        |                        |         |                   |
| 0   | taking pa   | rt in the hands-on e    | exercises and       | submitting a    | repo   | ort, passing the exar  | ninati  | lon.              |
| 8   | This mod    | ule is used in the f    | ollowing degi       | ree programn    | nes a  | is well                |         |                   |
| 0   | INOME       |                         | 1                   |                 |        |                        |         |                   |
| 9   |             | grade on total grad     | le                  |                 |        |                        |         |                   |
| 10  | 0/11/       | hility for modulo       |                     |                 |        |                        |         |                   |
| 10  | PD Dr h     | abil Rebecca Ianisc     | ĥ                   |                 |        |                        |         |                   |
| 11  | Other inf   | ormation                | .11                 |                 |        |                        |         |                   |
| 11  | Lecture n   | otes will be provide    | .d.                 |                 |        |                        |         |                   |
|     | Lecture II  | oles will be provide    | .u.                 |                 |        |                        |         |                   |

| ADV | ADVANCED ATOMISTIC SIMULATION METHODS |                       |  |                   |             |                         |        |                   |  |  |
|-----|---------------------------------------|-----------------------|--|-------------------|-------------|-------------------------|--------|-------------------|--|--|
| Mod | ule code                              | Student               | Credits                                    | Semeste           | er          | Frequency               |        | Duration          |  |  |
|     | 7.13                                  | workload              | 6 ECTS                                     | 3rd               |             | winter term             |        | 1 semester        |  |  |
| 1   | Types of                              | 180 nours             | Contact h                                  | 01179             | Inc         | lonondont study         | Clar   |                   |  |  |
| 1   | a) lecture                            | louises.              | a) 30 hrs (                                | 2 SW/S            | 120         | ) hours                 | 20 s   | tudents           |  |  |
|     | b) classes                            | focusing on hands     | $a_{1} = 50 \text{ ms}$ (s-<br>b) 30 hrs ( | b) 30 hrs (2 SWS) |             | 5 110015                | 203    | luuciits          |  |  |
|     | on compi                              | itational tasks       | <i>b)</i> 50 ms (                          | 201101            |             |                         |        |                   |  |  |
| 2   | Learning                              | outcomes              |  |                   |             |                         |        |                   |  |  |
|     | The stude                             | ents gain fundame     | ntal knowledge                             | of techniqu       | ies a       | nd methods used in      | adva   | nced atomistic    |  |  |
|     | simulatio                             | ns that address lar   | ge system sizes                            | s, long-time      | scale       | es, and long-range i    | nterac | ctions. They can  |  |  |
|     | classify si                           | mulation methods      | including mol                              | ecular static     | s, m        | olecular dynamics a     | and M  | Ionte Carlo sim-  |  |  |
|     | ulations, a                           | and apply appropri    | ate models of i                            | nteratomic        | inter       | cactions (DFT, tight    | bindi  | ng, empirical     |  |  |
|     | potentials                            | s). The students can  | n evaluate the v                           | alidity of th     | e sin       | nulation outcomes a     | and th | neir relation to  |  |  |
|     | measurab                              | ole material proper   | ties for several                           | case studies      | . Th        | e students are able t   | o pla  | n, execute and    |  |  |
|     | monitor a                             | atomistic simulatio   | ns.  |                   |             |                         |        |                   |  |  |
| 3   | Subject ai                            | ims                   |  |                   |             |                         |        |                   |  |  |
|     | • (                                   | Generation, analysi   | s and optimiza                             | tion of atom      | nic st      | tructures               |        |                   |  |  |
|     | • N                                   | Molecular statics ar  | nd relaxation al                           | gorithms          |             |                         |        |                   |  |  |
|     | • 1                                   | Molecular dynamic     | s in various en                            | sembles, the      | ermo        | ostats                  |        |                   |  |  |
|     | • N                                   | Monte Carlo metho     | ds, spin lattice                           | models, tra       | nsiti       | on state theory         |        |                   |  |  |
|     | • A                                   | Accelerated techniq   | ues and hybrid                             | l approaches      | 5           |                         |        |                   |  |  |
|     | • F                                   | Rigorous coarse-gra   | aining of atomi                            | c interaction     | n mo        | odels                   |        |                   |  |  |
|     | • \                                   | Workflows for atom    | nistic simulatio                           | ns                |             | <b>C</b> 1              |        |                   |  |  |
|     | • (                                   | Case studies: e.g. el | asticity and ph                            | onons, diffu      | ision       | i, ferroelectricity, me | elting |                   |  |  |
| 4   | Teaching                              | methods               |  |                   |             |                         |        |                   |  |  |
| -   | lecture, ex                           | xercises              |  |                   |             |                         |        |                   |  |  |
| 5   | backgroup                             | nd in physical chor   | on<br>Digtag or rolato                     | d diaciplina      | lano        | wladge of linux luni    | w onv  | ironmont and      |  |  |
|     | Dackgrou                              | '/Fortran program     | ming language                              | a aiscipiine,     | KIIO        | wiedge of fillux/ull    | IX env | iroiiiiieiit allu |  |  |
|     | narticinat                            | ion in "advanced n    | umerical meth                              | s<br>Inds: atomis | tic si      | imulation methods"      | or si  | milar course      |  |  |
| 6   | Assessme                              | ent methods           | uniencai metri                             |                   |             | initiation methods      | 01 51  | iiiiai course.    |  |  |
| Ŭ   | oral (0.5 k                           | nours) or written (2  | hours) examir                              | nation. Boni      | is po       | oints can be gained l   | ov sul | omitting solu-    |  |  |
|     | tions to th                           | ne problem sheets     | that are distrib                           | uted in class     | ло ре<br>5. | Sinto can de Gamea      |        | Summering South   |  |  |
| 7   | Prerequis                             | ites for the assign   | nent of credit I                           | points            |             |                         |        |                   |  |  |
|     | passing th                            | ne exam (bonus po     | ints will be tak                           | en into acco      | unt)        |                         |        |                   |  |  |
| 8   | This mod                              | ule is used in the f  | ollowing degre                             | e programn        | nes a       | ıs well                 |        |                   |  |  |
|     | none                                  |                       |  |                   |             |                         |        |                   |  |  |
| 9   | Impact of                             | f grade on total gra  | de   |                   |             |                         |        |                   |  |  |
|     | 6/117                                 |                       |  |                   |             |                         |        |                   |  |  |
| 10  | Responsi                              | bility for module     |  |                   |             |                         |        |                   |  |  |
|     | Prof. Dr.                             | Anna Grünebohm        | and Dr. Matou                              | is Mrovec         |             |                         |        |                   |  |  |
| 11  | Other inf                             | ormation              |  |                   |             |                         |        |                   |  |  |
|     | -                                     |                       |  |                   |             |                         |        |                   |  |  |

| COM | COMPUTATIONAL FRACTURE MECHANICS |                        |                  |                         |        |                       |        |                   |  |  |
|-----|----------------------------------|------------------------|------------------|-------------------------|--------|-----------------------|--------|-------------------|--|--|
| Mod | lule code                        | Student                | Credits          | Semester                | r      | Frequency             |        | Duration          |  |  |
|     | 7.14                             | workload               | 6 ECTS           | 3rd                     |        | winter term           |        | 1 semester        |  |  |
|     |                                  | 180 hours              |                  |                         |        |                       |        |                   |  |  |
| 1   | Types of o                       | courses:               | Contact h        | ours                    | Ind    | lependent study       | Cla    | ss size           |  |  |
|     | a) lecture                       |                        | a) 30 hrs (      | 2 SWS)                  | 120    | ) hours               | a) 2   | 0 students        |  |  |
|     | b) class                         |                        | b) 30 hrs (      | 2 SWS)                  |        |                       | b) 1   | 0 students        |  |  |
| 2   | Learning                         | outcomes               |                  | .1 . 1                  | c      |                       |        | C · 1             |  |  |
|     | The stude                        | nts attain the abilit  | y to independe   | ently simulat           | te fra | acture including pla  | sticit | y for a wide      |  |  |
|     | range of r                       | naterials and geom     | etries. Based o  | on the acquir           | ed u   | inderstanding of the  | e diff | erent types of    |  |  |
|     | brittle fra                      | cture and ductile fai  | lure of mater    | ials, they are          | ena    | bled to choose appro  | opria  | te fracture mod-  |  |  |
|     | els and to                       | implement them in      | i a finite elem  | transa of from          | nen    | t. They gain sufficie |        | iowiedge about    |  |  |
|     | indopond                         | encal Dackground of    | oring lovel th   | o students d            | iacri  | minate between git    | le Tel | evallt illerature |  |  |
|     | in a struc                       | ture or component      | can be tolerate  | e students d            | whic   | h conditions cracks   | atio   | not admissible    |  |  |
|     | respectively.                    |                        |                  |                         |        |                       |        |                   |  |  |
| 3   | Subject ai                       | ms                     |                  |                         |        |                       |        |                   |  |  |
|     | • F                              | henomenology of f      | racture/Fractu   | are on the at           | omi    | c scale               |        |                   |  |  |
|     | • (                              | Concepts of linear el  | astic fracture   | mechanics               |        |                       |        |                   |  |  |
|     | • (                              | Concepts of elastic-p  | lastic fracture  | mechanics               |        |                       |        |                   |  |  |
|     | • F                              | curve behavior of      | materials        |                         |        |                       |        |                   |  |  |
|     | • (                              | Concepts of cohesive   | zones (CZ),      | extended fin            | ite e  | lements (XFEM) an     | d dai  | mage mechanics    |  |  |
|     | • F                              | inite element mode     | eling of fractu  | re for static a         | ind o  | dynamic cracks        |        |                   |  |  |
|     | • A                              | Application to brittle | fracture & du    | actile failure          | for o  | different geometries  | and    | loading situa-    |  |  |
|     | t                                | ions                   |                  |                         |        |                       |        |                   |  |  |
| 4   | Teaching                         | methods                |                  |                         |        |                       |        |                   |  |  |
|     | lecture, h                       | ands-on classes, mi    | ni-project incl  | . seminar tal           | k, a   | ssignments            |        |                   |  |  |
| 5   | Prerequis                        | ites for participation | n<br>            |                         |        |                       |        |                   |  |  |
| -   | basic kno                        | wledge about solid     | mechanics an     | d plasticity is         | s rec  | commended             |        |                   |  |  |
| 6   | Assessme                         | ent methods            |                  |                         |        | 1 10 1                |        |                   |  |  |
|     | Portfolio                        | exam including rep     | orts on assign   | ments, semi             | nar    | and self-evaluation   | repo   | rt                |  |  |
| 7   | Prerequis                        | ites for the assignm   | ient of credit j | points                  |        |                       |        |                   |  |  |
| 0   | passing fi                       | nai module examin      | ation            |                         |        |                       |        |                   |  |  |
| ð   | Computer                         | tional Engineering     | Master course    | e programm<br>Naschinor | les a  | is well               |        |                   |  |  |
| 0   | Impact of                        | arado on total arad    |                  |                         | IDat   | ł                     |        |                   |  |  |
| ,   | 6/117                            | grade on total grad    | C                |                         |        |                       |        |                   |  |  |
| 10  | Responsi                         | vility for module      |                  |                         |        |                       |        |                   |  |  |
| 10  | Prof. Dr.                        | Alexander Hartmai      | er               |                         |        |                       |        |                   |  |  |
| 11  | Other inf                        | ormation               | -                |                         |        |                       |        |                   |  |  |
|     | Lecture n                        | otes will be provide   | d.               |                         |        |                       |        |                   |  |  |

| ADVANCED STATISTICAL METHODS IN MATERIALS SCIENCE |                    |   |                     |                 |        |                         |        |                    |  |
|---|--------------------|---|---------------------|-----------------|--------|-------------------------|--------|--------------------|--|
| Mod   | ule code           | Student work-                             | Credits             | Semester        | 1      | Frequency               |        | Duration           |  |
|   | 7.15               | load                                      | 6 ECTS              | 3rd             |        | winter term             |        | 1 semester         |  |
|   | -                  | 180 hours                                 |                     |                 |        |                         | -      |                    |  |
| 1   | Types of o         | courses                                   | Contact             | hours           | Inc    | lependent study         | Cla    | ss size            |  |
|   | a) lecture         |   | a) 45 hrs           | (2 SWS)         | 120    | ) hours                 | a) 1   | 5 students         |  |
|   | b) class           |   | b) 15 hrs           | s (1 SWS)       |        |                         | b) 1   | 5 students         |  |
| 2   | Learning           | outcomes                                  |                     |                 |        |                         |        |                    |  |
|   | After part         | icipating in the m                        | odule student       | S               |        |                         |        |                    |  |
|   | • r                | emember a variety                         | of uncertaint       | ty indication r | neth   | ods, their limitation   | is and | d applicability    |  |
|   | • a                | pply active learnin                       | g and Bayesia       | in optimizatio  | on m   | ethods to materials     | prop   | erties optimiza-   |  |
|   | t                  | ion problems                              | 11                  | C 1             |        |                         |        |                    |  |
|   | • C                | onstruct deep gen                         | erative model       | s for material  | s pro  | operties generation     |        |                    |  |
|   | • a                | ssess limitations a                       | nd applicabili      | ity of these me | etho   | ds and select proper    | met    | hods for particu-  |  |
|   | • 6                | reate Python code                         | to implement        | t and use aboy  | ve-m   | entioned methods t      | o sol  | ve simple prob-    |  |
|   | le                 | ems                                       | to implement        | t allu use abov | vC-111 | ientioned methods (     | 0 301  | ve simple prob-    |  |
| 3   | Subject ai         | ims                                       |                     |                 |        |                         |        |                    |  |
|   | • P                | Probability distribu                      | tions and Bay       | esian statistic | S      |                         |        |                    |  |
|   | • T                | <b>Uncertainty indicat</b>                | ion and quan        | tification      |        |                         |        |                    |  |
|   | • E                | Bayesian optimizat                        | ion                 |                 |        |                         |        |                    |  |
|   | • A                | Active learning                           |                     |                 |        |                         |        |                    |  |
|   | • (                | Generative models                         | (neural netwo       | orks - auto-en  | code   | rs, generative adver    | saria  | l networks, etc.)  |  |
| 4   | Teaching           | methods                                   |                     |                 |        |                         |        |                    |  |
|   | lecture, cl        | asses including ha                        | nds-on exerci       | ises with Pyth  | on a   | nd Jupyter notebool     | k, mi  | ni project         |  |
| 5   | Prerequis          | ites for participation                    | on                  | ( , , 1 T C     |        | · " 1"D · 1 ·           |        | 1 .                |  |
|   | Successful         | il completion of th                       | e modules "M        | laterials Infor | mat    | ics" and "Data-drive    | n ma   | iterials science – |  |
| 6   |                    | nt methods                                | ienaea.             |                 |        |                         |        |                    |  |
| Ŭ   | Completie          | on of mini project                        | with written 1      | project report  |        |                         |        |                    |  |
| 7   | Prerequis          | ites for the assign                       | nent of credit      | t points        |        |                         |        |                    |  |
|   | Accepted           | project report                            |                     | 1               |        |                         |        |                    |  |
| 8   | This mod           | ule is used in the f                      | following deg       | ree programn    | nes a  | ıs well                 |        |                    |  |
|   | None               |   |                     |                 |        |                         |        |                    |  |
| 9   | Impact of          | grade on total gra                        | de                  |                 |        |                         |        |                    |  |
| 10  | 6/117<br>Decreanti | h:1:                                      |                     |                 |        |                         |        |                    |  |
| 10  | Responsi           | Dility for module                         | veggorghin          |                 |        |                         |        |                    |  |
| 11  | Other info         | ormation                                  | ysogoiskiy          |                 |        |                         |        |                    |  |
| 11  | Literature         |   |                     |                 |        |                         |        |                    |  |
|   | • T                | . Hastie, R. Tibshi                       | rani. I. Friedi     | man: The Eler   | men    | ts of Statistical Lear  | ning:  | Data Mining.       |  |
|   | I                  | nference, and Pred                        | liction, Sprin      | ger (2009);     |        |                         | 8.     |                    |  |
|   | • A                | A. Gelman, J. B. Ca                       | rlin, H. S. Ste     | ern, D. B. Dur  | nson   | , A. Vehtari, D. B. R   | ubin   | : Bayesian Data    |  |
|   |                    | Malysis, Chapman                          | and Hall/CR         | C (2013);       | C.     | tatistics in Duthers (? | )nd c  | d) O'Bailler       |  |
|   |                    | Jowney, Allen B. (A                       | 2021). I mink l     | Dayes: Bayesia  | 411 Sl | austics in Python (2    | ind e  | u.j. U Keilly.     |  |
|   |                    | Oster D. Generativ<br>D'Reilly Media, 201 | e deep learni<br>9. | ng: teaching i  | nach   | lines to paint, write,  | , com  | pose, and play. –  |  |
|   | • J                | . VanderPlas: Pyth<br>D'Reilly (2016)     | on Data Scier       | nce Handbook    | c: Es  | sential Tools for Wo    | orking | g with Data,       |  |



| SUR | FACE SO     | CIENCE AND C           | ORROSION         |                |        |                                       |            |                    |
|-----|-------------|------------------------|------------------|----------------|--------|---------------------------------------|------------|--------------------|
| Mod | lule code   | Student                | Credits          | Semeste        | r      | Frequency                             |            | Duration           |
|     | 7.16        | workload               | 6 ECTS           | 3rd            |        | winter term                           |            | 1 semester         |
|     |             | 180 hours              |                  |                | -      |                                       |            |                    |
| 1   | Types of o  | courses:               | Contact he       | ours           | Inc    | aependent study Cla                   |            | ss size            |
|     | a) lecture  |                        | a) 45 hrs (.     | 3 SWS)         | 120    | ) hours                               | a) 2       | 5 students         |
| 2   | b) class    |                        | b) 15 hrs (      | I SWS)         |        |                                       | D) 2       | 25 students        |
| 2   | Learning    | outcomes               |                  |                |        | · · · · · · · · · · · · · · · · · · · |            | 1                  |
|     | Students    | will gain a fundam     | iental understa  | naing of cor   | rosi   | on science, from da                   | sic ei     | ectrochemistry     |
|     | or nomog    | eneous metal corre     | They will mean   | a aspects of   | local  | lized corrosion, as v                 | ven a      | s of complex       |
|     | compone     | nts and structures.    | I ney will men   | norize the ba  | asics  | s of applied surface                  | techn      | Furth array are    |
|     | the are ab  | lo to rolato thoir kr  | nuung an oun     | ook of flovel  | noct   | a of matorials soloci                 | ion i      | . Fulliennoie,     |
|     | sion dam    | age and measures       | for counteracti  | gilleetilig as | speci  | S OI IIIateriais seleci               | .1011, 6   | analysing corro-   |
| 3   | Subject a   | age and measures       |                  |                | 1.     |                                       |            |                    |
| 5   |             | hort introduction i    | nto surface sci  | ence and ele   | octro  | chemistry                             |            |                    |
|     | • f         | indamental aspect      | s of corrosion   | crience, the   | rmo    | dynamics and kinet                    | ics (P     | ourbaix dia-       |
|     | • 1         | rams Butler-Volm       | er equation etc  | ~              | 11100  | aynamics and kinet                    |            | Ourbaix uia-       |
|     | e r         | assivity of materia    | lei equation ett |                |        |                                       |            |                    |
|     | • +         | vnical corrosion pr    | oblems such a    | s atmosphe     | ric co | orrosion himetal co                   | rrosi      | on localised cor-  |
|     | r           | osion corrosion il     | nder biofilms 1  | basics of hig  | h te   | mperature corrosio                    | 11031<br>1 | on, iocanscu coi   |
|     | • r         | naterials choices b    | ased on applica  | tion require   | mer    | ts (such as corrosiv                  | enes       | s of the environ.  |
|     | r           | nent)                  | ased on applied  | non require    |        | 113 (30011 83 0011031)                | CIICS      |                    |
|     | • 0         | ountermeasures a       | painst corrosio  | n. such as b   | v ele  | ctrochemical corros                   | ion n      | protection, by im- |
|     | r           | proved construction    | , metallic, inor | ganic and o    | rgan   | ic coatings and rela                  | ted p      | re-treatments.     |
|     | i i         | nhibitors              | -,,              | 8              | -8     |                                       | ···· r     |                    |
|     | • e         | valuation of corros    | sion damage      |                |        |                                       |            |                    |
|     | • 0         | ounteracting meth      | ods best to use  | for differen   | it cas | ses                                   |            |                    |
| 4   | Teaching    | methods                |                  |                |        |                                       |            |                    |
|     | lecture, cl | ass, including a sh    | ort lab course   |                |        |                                       |            |                    |
| 5   | Prerequis   | ites for participation | on               |                |        |                                       |            |                    |
|     | successfu   | l completion of "St    | tatistical Mecha | anics and Fu   | ında   | mental Materials Pl                   | nysic      | s" (2c) and        |
|     | "Element    | s of Microstructure    | e" (2a) recomm   | ended.         |        |                                       |            |                    |
| 6   | Assessme    | ent methods            |                  |                |        |                                       |            |                    |
|     | written ex  | amination (2 hour      | rs)              |                |        |                                       |            |                    |
| 7   | Prerequis   | ites for the assign    | nent of credit p | points         |        |                                       |            |                    |
|     | passing th  | ne written examina     | tion             |                |        |                                       |            |                    |
| 8   | This mod    | ule is used in the f   | following degre  | e programn     | nes a  | ıs well                               |            |                    |
|     | Master of   | Science in Mecha       | nical Engineeri  | ng: Werksto    | off-E  | ngineering                            |            |                    |
| 9   | Impact of   | grade on total gra     | de               |                |        |                                       |            |                    |
|     | 6/117       |                        |                  |                |        |                                       |            |                    |
| 10  | Responsi    | bility for module      |                  |                |        |                                       |            |                    |
|     | Prof. Dr.   | rer. nat. Martin Str   | atmann, Dr. re   | er. nat. Mich  | ael I  | Rohwerder                             |            |                    |
| 11  | Other info  | ormation               |                  |                |        |                                       |            |                    |
|     | Lecture n   | otes will be provide   | ed.              |                |        |                                       |            |                    |

| MATERIALS FOR AEROSPACE APPLICATIONS |                    |                        |                  |                       |                |                        |        |                       |  |
|--------------------------------------|--------------------|------------------------|------------------|-----------------------|----------------|------------------------|--------|-----------------------|--|
| Mod                                  | ule code           | Student                | Credits          | Semeste               | r              | Frequency              |        | Duration              |  |
|                                      | 7.17               | workload               | 6 ECTS           | 3rd                   |                | winter term            |        | 1 semester            |  |
|                                      |                    | 180 hours              |                  |                       |                |                        |        |                       |  |
| 1                                    | Types of o         | courses:               | Contact he       | ours                  | Ind            | dependent study Cla    |        | ss size               |  |
|                                      | a) lecture         | 2                      | a) 45 hrs (      | a) 45 hrs (3 SWS) 120 |                | ) hours                | a) 2   | 25 students           |  |
| -                                    | b) class           |                        | b) 15 hrs (      | 1 SWS)                |                |                        | b) 2   | 25 students           |  |
| 2                                    | Learning           | outcomes               |                  | C 1. : . 1 C          |                |                        |        |                       |  |
|                                      | Students           | gain a comprehens      | ive overview o   | of high perio         | orma           | ance materials for a   | erosp  | bace applications,    |  |
|                                      | which inc          | iudes the well-intro   | aucea materia    | ais and mate          | riai           | systems as well as n   | ew a   | levelopments and      |  |
|                                      | visionary          | concepts. They und     | arstand now      | materials al          | ia n<br>fotia  | naterial systems are   | aesi   | igned to be light     |  |
|                                      | anu renat          | onte under extreme s   | can catogorize   | the degrad            | tion           | ue loading, night ter  | nper   | atures, and loarn how |  |
|                                      | characteri         | ization and testing r  | call categorize  | end for quali         | fvin           | a materials and join   | te foi | r perospace appli-    |  |
|                                      | cations T          | hev are able to appl   | v concepts and   | d methods f           | rynn<br>Sr lif | fetime assessment      | 15 10  | actospace appli-      |  |
| 3                                    | Subject a          | ms                     | y concepts un    | a methods i           | <i>J</i> 1 111 | etille ussessillent.   |        |                       |  |
| 5                                    | • 1                | oading conditions f    | or componen      | ts of air- and        | sna            | ce crafts (structures  | and    | engines)              |  |
|                                      | • 1                | )evelopment of mat     | erials and ma    | terial system         | is fo          | r specific service co  | nditi  | ons in aerospace      |  |
|                                      |                    | polications (e.g. for  | aero-engines     | rocket engi           | nes            | thermal protection     | shiel  | ds for re-entry       |  |
|                                      | v                  | ehicles, light weigh   | t structures fo  | r airframes.          | win            | gs, and satellites)    | Sinci  | us for re entry       |  |
|                                      | • T                | Degradation and day    | nage mechani     | isms of aero          | snac           | e materials and mat    | erial  | systems under         |  |
|                                      | s                  | ervice conditions      | inge meenum      | 191119 01 d010        | Pue            |                        |        |                       |  |
|                                      | • (                | Characterization and   | l testing meth   | ods for mate          | erial          | s and joints for aero  | space  | e applications        |  |
|                                      | • (                | Concepts and metho     | ds for lifetime  | e assessmen           | t. In          | troduction to conce    | pts of | f mechanical          |  |
|                                      | p                  | properties of materia  | als (stress-stra | in curves, st         | iffne          | ess, strength, ductili | ty)    |                       |  |
| 4                                    | Teaching           | methods                |                  |                       |                |                        | .,     |                       |  |
|                                      | lecture, cl        | ass                    |                  |                       |                |                        |        |                       |  |
| 5                                    | Prerequis          | ites for participation | n                |                       |                |                        |        |                       |  |
|                                      | backgrou           | nd in materials scie   | nce, mechanio    | cal engineer          | ng,            | physics or related di  | iscipl | line                  |  |
| 6                                    | Assessme           | ent methods            |                  |                       |                |                        |        |                       |  |
|                                      | written (2         | hours) or oral (0.5    | hours) examir    | nation, depe          | ndin           | ig on number of stu    | dent   | S                     |  |
| 7                                    | Prerequis          | ites for the assignm   | ent of credit p  | points                |                |                        |        |                       |  |
|                                      | passing th         | ne exam                |                  |                       |                |                        |        |                       |  |
| 8                                    | This mod           | ule is used in the fo  | llowing degre    | e programn            | ies a          | is well                |        |                       |  |
|                                      | Master of          | Science in Mechan      | ical Engineeri   | ng: Werksto           | tt-E           | ngineering             |        |                       |  |
|                                      | Master of          | Science in Comput      | ational Engin    | eering                |                |                        |        |                       |  |
| 9                                    | Impact of          | grade on total grad    | e                |                       |                |                        |        |                       |  |
| 10                                   | 0/11/<br>Decrease: | h:1: for modulo        |                  |                       |                |                        |        |                       |  |
| 10                                   | Responsi           | Duity for module       | 2                |                       |                |                        |        |                       |  |
| 11                                   | Other inf          | nig. Warton Dartsch    | l                |                       |                |                        |        |                       |  |
| 11                                   | Locture n          | otog will be provide   | donling          |                       |                |                        |        |                       |  |
| 1                                    | Lecture n          | oles will be provide   | a omme.          |                       |                |                        |        |                       |  |

| Mod | lule code   | Student                  | Credits           | Semester       | Frequency               |        | Duration          |
|-----|-------------|--------------------------|-------------------|----------------|-------------------------|--------|-------------------|
|     | 7.18        | workload                 | 6 ECTS            | 3rd            | winter term             |        | 1 semester        |
|     |             | 180 hours                |                   |                |                         |        |                   |
| 1   | Types of o  | courses:                 | Contact he        | ours           | Independent study       | Cla    | ss size           |
|     | a) lecture  |                          | a) 30 hrs (2      | 2 SWS)         | 120 hours               | a) 1   | 5 students        |
|     | b) exercise | es                       | b) 30 hrs (       | 2 SWS)         |                         | b) 1   | 5 students        |
| 2   | Learning    | outcomes                 |                   |                |                         |        |                   |
|     | By comple   | eting the course, st     | udents gain in    | sight into a r | ange of three-dimensi   | onal r | nanoscale and     |
|     | atomic sc   | ale material charac      | terization tech   | niques, e.g. 3 | D x-ray microscopy, el  | lectro | n tomography      |
|     | and atom    | probe tomography         | . They can des    | cribe the wor  | king principles of eacl | h tech | nique in detail,  |
|     | summariz    | ze applications in a     | vast of applica   | tions, such a  | s engineering alloys, c | atalys | t materials, sem- |
|     | iconducto   | rs, etc. and solve so    | cientific questi  | ons related to | material science by u   | sing t | hree-dimen-       |
|     | sional ma   | terial characterizat     | ion techniques    | . Additionall  | y, students will unders | stand  | three-dimen-      |
|     | sional nai  | noscale and atomic       | scale material    | characteriza   | tion methods, which a   | re cur | rently extremely  |
|     | important   | t in Doth industry a     | ind academia, a   | and achieve s  | ome basic nands-on ex   | xperie | ence on sample    |
|     | preparatio  | m and sample ana         | lysis on one of   | these technic  | lues (depends on the a  | ivanai | bility of instru- |
| 2   | Subject a   | ma                       |                   |                |                         |        |                   |
| 3   | Subject al  | IIIS<br>D Enorm dianorai | V rou apoctr      | aconu          |                         |        |                   |
|     | • 3         | D Eilergy-uispersio      | ve A-ray specific | oscopy         |                         |        |                   |
|     | • 5         | tom probe tomogr         | scopy<br>saby     |                |                         |        |                   |
|     | • P         | loctron tomograph        | арпу              |                |                         |        |                   |
|     |             | rectron tomograph        | ly                |                |                         |        |                   |
|     |             | clay tollography         | licing/sconnin    | a oloctron m   | icroscopy               |        |                   |
| 4   | Teaching    | methods                  | sitcing/scattini  | ig election in | icroscopy               |        |                   |
| 4   | lecture ex  | vercises                 |                   |                |                         |        |                   |
| 5   | Prerequis   | ites for participatio    | n .               |                |                         |        |                   |
| 5   | none        | nes for participatio     | /11               |                |                         |        |                   |
| 6   | Assessme    | ent methods              |                   |                |                         |        |                   |
| U   | During th   | e semester each st       | udent will be a   | ssigned a cu   | rent topic on which th  | ne stu | dent has to write |
|     | a five-pag  | e report and give a      | talk.             | ssigned a ca   |                         | 10 500 |                   |
| 7   | Prerequis   | ites for the assignr     | nent of credit r  | ooints         |                         |        |                   |
|     | Submissi    | on of report and ho      | olding of semir   | ar talk        |                         |        |                   |
| 8   | This mod    | ule is used in the f     | ollowing degre    | e programm     | es as well              |        |                   |
|     | Masters N   | Aechanical Enginee       | ering: Werksto    | ff-Engineerir  | ıg                      |        |                   |
| 9   | Impact of   | grade on total grad      | de                | 0              | v                       |        |                   |
|     | 6/117       | 0                        |                   |                |                         |        |                   |
| 10  | Responsi    | bility for module        |                   |                |                         |        |                   |
|     | Prof. Dr.   | Tong Li                  |                   |                |                         |        |                   |
| 11  | Other info  | ormation                 |                   |                |                         |        |                   |
|     | -           |                          |                   |                |                         |        |                   |



| Modu | ıle code                        | Student               | Credits           | Semester         |                | Frequency            |        | Duration            |
|------|---------------------------------|-----------------------|-------------------|------------------|----------------|----------------------|--------|---------------------|
|      | 7.19                            | workload              | 6 ECTS            | 3rd              |                | winter term          |        | 1 semester          |
|      |                                 | 180 hours             |                   |                  |                |                      |        |                     |
| 1    | Types of o                      | courses:              | Contac            | hours            | Ind            | lependent study      | Cla    | ss size             |
|      | a) lecture                      | + group seminar       | a) 30 hi          | rs (2 SWS)       | 120            | ) hours              | a) 1   | 0 students          |
|      | b) practica                     | al studies            | b) 30 hi          | rs (2 SWS)       |                |                      | b) 1   | 10 students         |
| 2    | Learning                        | outcomes              |                   |                  |                |                      |        |                     |
|      | Students                        | are able to formula   | ite and desci     | ribe the found   | lation         | s of electronic stru | cture  | calculations.       |
|      | This will i                     | Include the transla   | tion of the q     | uantum mec       | hanica         | al equations into p  | seudo  | code that may       |
|      | then be in                      | nplemented in con     | nputer code       | . They will be   | able t         | to use and implement | ent th | e most common       |
|      | to apprais                      | a solvers that are en | mpioyea in o      | quantum med      | name<br>ulatio | ai problems. In un   | us way | so be enabled to    |
|      | choose th                       | e most appropriate    | electronic s      | tructure com     | nutati         | ional method and i   | mnlei  | so be ellabled to   |
|      | given rese                      | e most appropriate    |                   |                  | Pulat          | ionai menioù allu l  | mpie   |                     |
| 3    | Subject ai                      | ms                    |                   |                  |                |                      |        |                     |
| 0    | • •                             | Numerical impleme     | entation and      | solution of a    | singl          | e particle Schrödin  | iger e | nuation (electron   |
|      | i                               | n an effective poter  | ntial)            | , portation of a | 511-61         | Particle Sellioan    | 801 0  | function (creection |
|      | • E                             | Basis sets, represen  | ,<br>tation of op | erators in a ba  | asis           |                      |        |                     |
|      | • F                             | Results, analysis an  | d visualizati     | on of electror   | nic str        | ucture calculations  | 5      |                     |
|      | • 1                             | Numerical converge    | ence              |                  |                |                      |        |                     |
|      | • P                             | lane-wave pseudo-     | potential m       | ethod (iterativ  | ve diag        | gonalization, self-c | onsist | ency)               |
|      | • 1                             | ight binding Meth     | od                |                  |                |                      |        |                     |
|      | • E                             | Bond-order potentia   | als               |                  |                |                      |        |                     |
|      | • S                             | pecial topics and a   | pplications       | (structural sta  | bility         | , magnetism).        |        |                     |
| 4    | Teaching                        | methods               |                   |                  |                |                      |        |                     |
|      | lecture, p                      | ractical studies and  | l group sem       | inars            |                |                      |        |                     |
| 5    | Prerequis                       | ites for participatio | on                | • • •            | <b>1</b>       | 1.1                  | D1     | • "•                |
|      | successfu                       | I completion of "Ir   | itroduction       | to Quantum I     | Mecha          | anics in Solid State | Phys   | ics" is recom-      |
| 6    | mended.                         | nt matheda            |                   |                  |                |                      |        |                     |
| U    | written                         | amination (1.5 hor    | ure)              |                  |                |                      |        |                     |
| 7    | Prerequie                       | ites for the assignt  | nent of cred      | it noints        |                |                      |        |                     |
| /    | positively                      | evaluated written     | report and p      | assing of eval   | m              |                      |        |                     |
| 8    | This mod                        | ule is used in the f  | following de      | pree program     | mes a          | ıs well              |        |                     |
| 0    | None                            | and is used in the I  |                   | 9 k              |                |                      |        |                     |
| 9    | Impact of                       | grade on total grad   | de                |                  |                |                      |        |                     |
| -    | 6/117                           | 8 8                   |                   |                  |                |                      |        |                     |
| 10   | Responsi                        | bility for module     |                   |                  |                |                      |        |                     |
|      | Prof. Dr.                       | Ralf Drautz, Prof. 1  | Dr. Jörg Neı      | ıgebauer         |                |                      |        |                     |
| 11   | Other information               |                       |                   |                  |                |                      |        |                     |
|      | Lecture notes will be provided. |                       |                   |                  |                |                      |        |                     |



| LAT | LATTICE BOLTZMANN MODELLING:  |   |                |                 |        |                       |        |                  |  |  |  |
|-----|---|---|----------------|-----------------|--------|-----------------------|--------|------------------|--|--|--|
| FRO | M SIMPL   | E FLOWS TO  | INTERFAC       |                 | N Pł   | HENOMENA              |        |                  |  |  |  |
| Mod | ule code  | Student work-   | Credits        | Semester        | r      | Frequency             |        | Duration         |  |  |  |
|     | 7.20  | load  | 6 ECTS         | 3rd             |        | winter term           |        | 1 semester       |  |  |  |
|     |   | 180 hours   |                |                 | r      |                       |        |                  |  |  |  |
| 1   | Types of o  | courses   | Contact        | hours           | Inc    | lependent study       | Cla    | ss size          |  |  |  |
|     | a) lecture  |   | a) 30 hrs      | (2 SWS)         | 120    | ) hours               | a) 1   | 0 students       |  |  |  |
|     | b) class  |   | b) 30 hrs      | (2 SWS)         |        |                       | b) 1   | 0 students       |  |  |  |
| 2   | Learning outcomes   |   |                |                 |        |                       |        |                  |  |  |  |
|     | On succes   | sstul completion of   | this module    | , students wil  | l rec  | all equations of hyd  | rodyr  | namics and their |  |  |  |
|     | solutions   | for simple cases su   | ich as hydros  | tatic pressure  | e in a | in ideal gas (barome  | tric f | ormula), planar  |  |  |  |
|     | Couette fl  | ow and the Poiseu   | ille flow. The | y can outline   | the    | lattice Boltzmann m   | letho  | d (LBM) and ap-  |  |  |  |
|     | ply a simple code for simulating flow via LBM. Using the above mentioned simple cases, the stu- |   |                |                 |        |                       |        |                  |  |  |  |
|     | nroblems  | dents will be able to examine the validity of the LBM code and also address a number of interesting |                |                 |        |                       |        |                  |  |  |  |
|     | ofliquids   | on solid surfaces   | w ioi piessui  | e unicicilee i  | II uiv | ops and then enviro   | mine   | ints and wetting |  |  |  |
| 3   | Subject ai  | ms  |                |                 |        |                       |        |                  |  |  |  |
| 5   | • I   | ntroduction to fluid  | dynamics o     | n the continu   | um     | level (Euler and Nav  | ier-S  | tokes equations) |  |  |  |
|     | • F   | Basics of the lattice   | Boltzmann n    | nethod (LBM)    | )      | lever (Buier und riu) | ier b  | tokes equations) |  |  |  |
|     | • 5   | imulation of multi  | phase fluids:  | drops, bubbl    | es     |                       |        |                  |  |  |  |
|     | • V   | Vetting   | priase marasi  | arops, 54661    | 0.0    |                       |        |                  |  |  |  |
| 4   | Teaching  | methods   |                |                 |        |                       |        |                  |  |  |  |
|     | lecture, gr   | roup work, case stu   | dies, discuss  | ions            |        |                       |        |                  |  |  |  |
| 5   | Prerequis   | ites for participatio   | n              |                 |        |                       |        |                  |  |  |  |
|     | familiarit  | y with computer pr  | ogramming      | (C, Fortran, o  | r equ  | uivalent)             |        |                  |  |  |  |
| 6   | Assessme  | ent methods   |                |                 |        |                       |        |                  |  |  |  |
|     | oral exam   | ination (0.5 hours)   |                |                 |        |                       |        |                  |  |  |  |
| 7   | Prerequis   | ites for the assignment   | nent of credit | t <b>points</b> |        |                       |        |                  |  |  |  |
|     | passing th  | ne exam (for active   | participation  | in the lecture  | e, bo  | nus points will be co | onsid  | ered)            |  |  |  |
| 8   | This mod  | ule is used in the f  | ollowing deg   | ree programn    | nes a  | ıs well               |        |                  |  |  |  |
|     | none  |   |                |                 |        |                       |        |                  |  |  |  |
| 9   | Impact of   | grade on total grad   | le             |                 |        |                       |        |                  |  |  |  |
| 10  | 6/11/   | 11. C 1 1   |                |                 |        |                       |        |                  |  |  |  |
| 10  | Responsi  | Fathallah Varaila   |                |                 |        |                       |        |                  |  |  |  |
| 11  | Other inf   |   |                |                 |        |                       |        |                  |  |  |  |
| 11  | Lecture n   | otes will be provide  | h              |                 |        |                       |        |                  |  |  |  |



| INTERATOMIC POTENTIALS |   |                              |                             |                    |               |                      |       |                   |  |  |
|------------------------|---|------------------------------|-----------------------------|--------------------|---------------|----------------------|-------|-------------------|--|--|
| Mod                    | lule code   | Student work-                | Credits                     | Semester           |               | Frequency            |       | Duration          |  |  |
|                        | 7.21  | load                         | 6 ECTS                      | 3rd                |               | winter term          |       | 1 semester        |  |  |
|                        | 1   | 180 hours                    |                             |                    |               |                      |       |                   |  |  |
| 1                      | Types of o  | courses                      | Contact                     | nours              | Ind           | lependent study      | Cla   | ss size           |  |  |
|                        | a) lecture  |                              | a) 30 hrs                   | (2 SWS)            | 120           | hours                | a) 1  | 0 students        |  |  |
|                        | b) exercis  | es                           | b) 30 hrs                   | (2 SWS)            |               |                      | b) 1  | 0 students        |  |  |
| 2                      | Learning  | outcomes                     |                             | 11.                |               | . 16 1               | 1     | <u> </u>          |  |  |
|                        | After participating in the module, students are able to understand fundamental concepts of intera-                                  |                              |                             |                    |               |                      |       |                   |  |  |
|                        | tomic pot   | entials based on th          | e electronic s              | tructure, on c     | lassi         | cal approaches and   | on n  | nachine-learning. |  |  |
|                        | I ney are a   | able to carry out ato        | the entropy                 | ations for var     | lous          | materials using int  | erato | mic potentials    |  |  |
| 2                      | Subject of  | aryze and interpret          | the outcome                 | 8.                 |               |                      |       |                   |  |  |
| 5                      | Subject al  | mis<br>regione of interatomi | cintoraction                |                    |               |                      |       |                   |  |  |
|                        |   | tropic structure ap          | provimations                | ,<br>(tight bindin | a bo          | nd order notential   | -)    |                   |  |  |
|                        | • clee  | sical potentials (Le         | proximations<br>nnard-Iones | embedded-at        | g, DC<br>2m/l | Finnis-Sinclair Ter  | soff) |                   |  |  |
|                        | Classical potentials (Lennard-Jones, embedded-atom/Finnis-Sincialr, Tersoff)     force fields (Amber Charmer BeavEE)                |                              |                             |                    |               |                      |       |                   |  |  |
|                        | • Torce fields (Amber, Charmin, KeaxFF)   |                              |                             |                    |               |                      |       |                   |  |  |
|                        | many-atom expansions/cluster expansions     machine learning potentials (neural networks, Caussian approximation potentials, memory |                              |                             |                    |               |                      |       |                   |  |  |
|                        | t   | ensor potentials, at         | omic-cluster                | expansion, m       | essa          | ge-passing and grai  | oh re | presentations)    |  |  |
|                        | • mag   | netism. charge-tra           | nsfer, polariz              | ation              | coou          | 90 Pubbing and Braj  |       | p105011001015)    |  |  |
|                        | • para  | ameterization and            | validation                  |                    |               |                      |       |                   |  |  |
|                        | • s   | imulation tools and          | d applications              | 5                  |               |                      |       |                   |  |  |
| d4                     | Teaching  | methods                      |                             |                    |               |                      |       |                   |  |  |
|                        | lecture, co   | omputer exercises            |                             |                    |               |                      |       |                   |  |  |
| 5                      | Prerequis   | ites for participation       | on                          |                    |               |                      |       |                   |  |  |
|                        | none  |                              |                             |                    |               |                      |       |                   |  |  |
| 6                      | Assessme  | ent methods                  |                             |                    |               |                      |       |                   |  |  |
|                        | individua   | l project and/or ora         | al examinatio               | n (0.5 hours),     | depe          | ending on size of cl | ass   |                   |  |  |
| 7                      | Prerequis   | ites for the assignr         | nent of credit              | points             |               | _                    |       |                   |  |  |
|                        | successfu   | l completion of pro          | oject / passing             | g of written ex    | ami           | nation               |       |                   |  |  |
| 8                      | This mod  | ule is used in the f         | ollowing deg                | ree programm       | ies a         | s well               |       |                   |  |  |
|                        | none  |                              |                             |                    |               |                      |       |                   |  |  |
| 9                      | Impact of   | grade on total grad          | de                          |                    |               |                      |       |                   |  |  |
| 10                     | 6/11/   |                              |                             |                    |               |                      |       |                   |  |  |
| 10                     | Dr Motor  |                              | habil Thoma                 | a Unmmora          | hmi           | 4+                   |       |                   |  |  |
| 1                      | Dr. Matous Mrovec, PD Dr. habil. Thomas Hammerschmidt   |                              |                             |                    |               |                      |       |                   |  |  |
| 11                     | Other inf   | ormation                     |                             |                    |               |                      |       |                   |  |  |



| GENERAL OPTION MODULE |   |   |                  |              |       |                     |      |            |  |  |
|-----------------------|---|---|------------------|--------------|-------|---------------------|------|------------|--|--|
| Mod                   | ule code  | Student   | Credits          | Semeste      | er    | Frequency           |      | Duration   |  |  |
|                       | 8   | workload  | 6 ECTS           | 1st          |       | free choice of      |      | 1 semester |  |  |
|                       |   | 180 hours   |                  |              |       | available module    | es   |            |  |  |
| 1                     | Types of o  | courses:  | Contact he       | ours         | Ind   | lependent study     | Clas | ss size    |  |  |
|                       | lecture an  | id class  | 60 hrs           |              | 120   | hours               |      |            |  |  |
| 2                     | Learning  | outcomes  |                  |              |       |                     |      |            |  |  |
|                       | By freely choosing lectures, the students can widen their skill and method spectrum according to          |   |                  |              |       |                     |      |            |  |  |
|                       | their personal interests.   |   |                  |              |       |                     |      |            |  |  |
| 3                     | Subject ai  | ims   |                  |              |       |                     |      |            |  |  |
|                       | • [   | Develop knowledge   | and skills in fi | elds beyond  | l eng | ineering and scienc | e    |            |  |  |
|                       | Deepen knowledge about specific topics in Materials Science and Simulation according to     own interests |   |                  |              |       |                     |      |            |  |  |
|                       | • Any module from a Master's course at RUB will be recognized. Some suggested courses                     |   |                  |              |       |                     |      |            |  |  |
|                       | a   | are listed under points 6 and 7 (Elective and Specialization Modules in MS). Courses from |                  |              |       |                     |      |            |  |  |
|                       | the RUB's main course catalogue and from the international course catalogue can be taken                  |   |                  |              |       |                     |      |            |  |  |
|                       | i   | nto account.  |                  |              |       |                     |      |            |  |  |
| 4                     | Teaching  | methods   |                  |              |       |                     |      |            |  |  |
|                       | see specif  | ic module descript  | ion              |              |       |                     |      |            |  |  |
| 5                     | Prerequis   | ites for participatio   | n                |              |       |                     |      |            |  |  |
|                       | none  |   |                  |              |       |                     |      |            |  |  |
| 6                     | Assessme  | ent methods   |                  |              |       |                     |      |            |  |  |
|                       | written or  | oral examination a  | as given in spe  | cific module | e des | cription            |      |            |  |  |
| 7                     | Prerequis   | ites for the assignm  | nent of credit p | oints        |       |                     |      |            |  |  |
|                       | passing th  | ne examination  |                  |              |       |                     |      |            |  |  |
| 8                     | This mod  | ule is used in the f  | ollowing degre   | e programn   | nes a | s well              |      |            |  |  |
|                       | see specif  | ic module descript  | ion              |              |       |                     |      |            |  |  |
| 9                     | Impact of   | grade on total grad   | le               |              |       |                     |      |            |  |  |
| 10                    | 6/117   |   |                  |              |       |                     |      |            |  |  |
| 10                    | Responsi  | bility for module   |                  |              |       |                     |      |            |  |  |
| 11                    | Prot. Dr.   | Alexander Hartmai   | er               |              |       |                     |      |            |  |  |
| 11                    | Other info  | ormation  |                  |              |       |                     |      |            |  |  |
|                       | -   |   |                  |              |       |                     |      |            |  |  |



| INDUSTRIAL INTERNSHIP |              |                             |  |                     |        |                        |          |  |  |  |
|-----------------------|--------------|-----------------------------|--|---------------------|--------|------------------------|----------|--|--|--|
| Mod                   | ule code     | Student                     | Credits                                | Semeste             | er     | Frequency              | tor      | Duration                               |  |  |
|                       | 0.1          | 180 hours                   | 0 EC15                                 | 510                 |        | summer and win         | ler      | 1 semester                             |  |  |
| 1                     | Types of     | courses:                    | Contact he                             | ours                | Inc    | lependent study        | Class    | s size                                 |  |  |
| -                     | practical    | work                        | 20 hours                               | Juis                | 160    | 0 hours                | 1 stu    | dent                                   |  |  |
|                       | 1            |                             |  |                     |        |                        |          |  |  |  |
| 2                     | Learning     | outcomes                    | ·                                      |                     |        |                        |          |  |  |  |
|                       | The stude    | ents gain an initial        | insight into ind                       | dustrial prac       | ctice, | , enabling them to a   | pply th  | ne skills they                         |  |  |
|                       | have learn   | ned thus far to real        | world problem                          | is. They leai       | m al   | pout various areas of  | activi   | ty within a                            |  |  |
|                       | company      | , which allows then         | n to assess the                        | requiremen          | ts of  | different tasks and    | use th   | is knowledge                           |  |  |
| 2                     | for their of | own purposes, part          | icularly in mak                        | ing informe         | ea ca  | ireer choices in a tar | getea    | manner.                                |  |  |
| 5                     | During th    | uus<br>oo siy week internsl | nin in a researd                       | h and devel         | onr    | ent department act     | ivitios  | must be                                |  |  |
|                       | related to   | one or more of the          | following field                        | li anu ucver<br>ls· | opin   |                        | livities | inust be                               |  |  |
|                       | • r          | naterials design or         | development                            |                     |        |                        |          |  |  |  |
|                       | • r          | naterials synthesis         | ······································ |                     |        |                        |          |  |  |  |
|                       | • r          | naterials testing           |  |                     |        |                        |          |  |  |  |
|                       | • r          | naterials selection         | in the product                         | developmer          | nt pro | ocess                  |          |  |  |  |
|                       | • r          | naterials processin         | g                                      | -                   | -      |                        |          |  |  |  |
|                       | • r          | naterials characteri        | sation                                 |                     |        |                        |          |  |  |  |
|                       | • r          | naterials simulation        | n                                      |                     |        |                        |          |  |  |  |
|                       | • r          | naterials related da        | ta science                             |                     |        |                        |          |  |  |  |
|                       | • 0          | other materials rela        | ted areas                              |                     |        |                        |          |  |  |  |
| 4                     | Teaching     | methods                     |  |                     |        |                        |          |  |  |  |
| _                     | 6 week in    | ternship in researc         | h and developi                         | ment depart         | men    | it of a materials scie | nce rel  | lated company                          |  |  |
| 5                     | Prerequis    | ites for participation      | n                                      |                     |        |                        |          |  |  |  |
| 6                     | none         | nt mothods                  |  |                     |        |                        |          |  |  |  |
| 0                     | Written r    | enort (12.20 pages)         | in the commo                           | n scientific        | form   | nat to be handed in    | two w    | eeks after the                         |  |  |
|                       | end of the   | e six week internsh         | in the commo                           | ii sciciitiic       | 10111  | iut, to be nunded in   |          | certs unter the                        |  |  |
| 7                     | Prerequis    | ites for the assignr        | nent of credit I                       | ooints              |        |                        |          |  |  |  |
|                       | Positive e   | valuation of the wr         | itten report, in                       | ternship co         | nfirr  | nation or reference    | letter c | of employer                            |  |  |
| 8                     | This mod     | lule is used in the f       | ollowing degre                         | e programn          | nes a  | as well                |          |  |  |  |
|                       | none         |                             |  |                     |        |                        |          |  |  |  |
| 9                     | Impact of    | f grade on total grad       | le                                     |                     |        |                        |          |  |  |  |
|                       | 6/117        |                             |  |                     |        |                        |          |  |  |  |
| 10                    | Responsi     | bility for module           |  |                     |        |                        |          |  |  |  |
| 11                    | Prot. Dr.    | Alexander Hartma            | ler                                    |                     |        |                        |          |  |  |  |
| 11                    | Other inf    | ormation                    | otod with the                          | orrean or 1:        |        | unomigon of DUD in     | o duro   | ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~ |  |  |
|                       | A workpl     | an must be coordin          | ialed with the G                       | Jorrespondi         | ug si  | upervisor at RUB in    | auvan    | .ce.                                   |  |  |

| DOC | DOCUMENTING AND COMMUNICATING SCIENCE 1  |                        |                  |               |                         |        |                   |  |  |  |
|-----|--|------------------------|------------------|---------------|-------------------------|--------|-------------------|--|--|--|
| Mod | ule code   | Student                | Credits          | Semeste       | r Frequency             |        | Duration          |  |  |  |
|     | 9a   | workload               | 3 ECTS           | 1st           | winter term             |        | 1 semester        |  |  |  |
|     |  | 90 hours               |                  |               |                         |        |                   |  |  |  |
| 1   | Types of o   | courses:               | Contact he       | ours          | Independent study       | Cla    | ss size           |  |  |  |
|     | a) lecture   |                        | a) 15 hrs (      | 1 SWS)        | 60 hours                | 30 s   | students          |  |  |  |
|     | b) class   |                        | b) 15 hrs (      | 1 SWS)        |                         |        |                   |  |  |  |
| 2   | Learning   | outcomes               |                  |               |                         |        |                   |  |  |  |
|     | Participar   | nts will learn how to  | o prepare diffe  | rent types of | f scientific documents. | Struct | tural elements of |  |  |  |
|     | different formats will be discussed. An introduction to scientific typesetting, plotting and graphic   |                        |                  |               |                         |        |                   |  |  |  |
|     | tools will be given. After successful participation, students know the basics about scientific writing |                        |                  |               |                         |        |                   |  |  |  |
|     | and can independently  |                        |                  |               |                         |        |                   |  |  |  |
|     | <ul> <li>choose an appropriate format for presenting numerical data</li> </ul>                         |                        |                  |               |                         |        |                   |  |  |  |
|     | • create appealing, publication-ready graphics, figures, and tables                                    |                        |                  |               |                         |        |                   |  |  |  |
|     | •  | create structured do   | ocuments usin    | g LaTeX for   | typesetting             |        |                   |  |  |  |
| 3   | Subject aims   |                        |                  |               |                         |        |                   |  |  |  |
|     | Structures, style, and types of scientific documents   |                        |                  |               |                         |        |                   |  |  |  |
|     | • LaTeX  |                        |                  |               |                         |        |                   |  |  |  |
|     | • (  | Graphics and image     | es               |               |                         |        |                   |  |  |  |
|     | • 4  | Assessment, structu    | iring, and visu  | alization sci | entific data            |        |                   |  |  |  |
| 4   | Teaching   | methods                |                  |               |                         |        |                   |  |  |  |
|     | Lecture a  | nd hands-on tutoria    | als in CIP-pool  |               |                         |        |                   |  |  |  |
| 5   | Prerequis  | ites for participatio  | n                |               |                         |        |                   |  |  |  |
|     | none   |                        |                  |               |                         |        |                   |  |  |  |
| 6   | Assessme   | ent methods            |                  |               |                         |        | 1                 |  |  |  |
|     | Hands-or   | assessment in CII      | pool: visualiz   | ing given so  | ientific data and embed | lding, | description in a  |  |  |  |
| 7   | Lalex do   | cument template        |                  |               |                         |        |                   |  |  |  |
| /   | Prerequis  | utes for the assigning | nent of credit p | Doints        |                         |        |                   |  |  |  |
| 0   | This mod   | valuation of the na    | allowing dogra   |               |                         |        |                   |  |  |  |
| 0   | none   | luie is used in the fo | bilowing degre   | e programm    | ies as well             |        |                   |  |  |  |
| 9   | Impact of  | grade on total grad    | le               |               |                         |        |                   |  |  |  |
| ĺ   | 3/117  | - 5- auc on total glat | *~               |               |                         |        |                   |  |  |  |
| 10  | Responsi   | bility for module      |                  |               |                         |        |                   |  |  |  |
|     | Prof. Dr.  | Anna Grünebohm.        | Prof. Dr. Mar    | kus Stricker  |                         |        |                   |  |  |  |
| 11  | Other inf  | ormation               |                  |               |                         |        |                   |  |  |  |
|     | -  |                        |                  |               |                         |        |                   |  |  |  |





| DOCUMENTING AND COMMUNICATING SCIENCE 2 |   |                       |                   |                |       |                       |        |                |  |
|---|---|-----------------------|-------------------|----------------|-------|-----------------------|--------|----------------|--|
| Mod                                     | ule code  | Student               | Credits           | Semeste        | r     | Frequency             |        | Duration       |  |
|   | 9b  | workload              | 3 ECTS            | 2nd            |       | summer term           |        | 1 semester     |  |
|   |   | 90 hours              |                   |                |       |                       |        |                |  |
| 1                                       | Types of o  | courses:              | Contact he        | ours           | Inc   | lependent study       | Cla    | ss size        |  |
|   | a) lecture  |                       | a) 15 hrs (       | 1 SWS)         | 60    | hours                 | 30 s   | students       |  |
|   | b) class  |                       | b) 15 hrs (       | 1 SWS)         |       |                       |        |                |  |
| 2                                       | 2 Learning outcomes   |                       |                   |                |       |                       |        |                |  |
|   | After successful participation, students can independently                                      |                       |                   |                |       |                       |        |                |  |
|   | perform literature research   |                       |                   |                |       |                       |        |                |  |
|   | • evaluate text from scientific journal publications w.r.t. formal scientific writing criteria, |                       |                   |                |       |                       |        |                |  |
|   | style, and information content  |                       |                   |                |       |                       |        |                |  |
|   | •   | prepare a short wri   | tten report on a  | a scientific t | opic  | in materials science  | 2      |                |  |
| _                                       | •   | present (oral & slid  | es) a literature  | survey on a    | curi  | rent topic in materia | ls sc  | ience.         |  |
| 3                                       | Subject aims  |                       |                   |                |       |                       |        |                |  |
|   | Literature research, citations, quotations, copyright issues, plagiarism                        |                       |                   |                |       |                       |        |                |  |
|   | Presenting and structuring a scientific topic   |                       |                   |                |       |                       |        |                |  |
|   | • (   | Dral presentation to  | ols               |                |       |                       |        |                |  |
| 4                                       | Teaching  | methods               | 1                 | 1              |       |                       |        |                |  |
|   | Lecture a   | nd hands-on tutoria   | als in CIP-pool   | , literature-r | evie  | w as independent st   | udy    |                |  |
| 5                                       | Prerequis   | ites for participatio | n                 |                |       |                       |        |                |  |
| 6                                       |   | nt mothoda            |                   |                |       |                       |        |                |  |
| 0                                       | Short wri   | tten report short o   | ral presentation  | n              |       |                       |        |                |  |
| 7                                       | Prerequis   | ites for the assign   | nent of credit r  | noints         |       |                       |        |                |  |
| <b>`</b>                                | Positive e  | valuation of the wr   | itten report (lit | erature rese   | arch  | on an individual to   | pic) a | and successful |  |
|   | presentat   | ion of the topic dur  | ing a mini syn    | nposium.       |       |                       | P10) ( |                |  |
| 8                                       | This mod  | ule is used in the f  | ollowing degre    | e programn     | ies a | s well                |        |                |  |
|   | none  |                       | 0 0               | 1 8            |       |                       |        |                |  |
| 9                                       | Impact of   | grade on total grad   | le                |                |       |                       |        |                |  |
|   | 3/117   | 0 0                   |                   |                |       |                       |        |                |  |
| 10                                      | Responsi  | bility for module     |                   |                |       |                       |        |                |  |
|   | Prof. Dr.   | Anna Grünebohm,       | Prof. Dr. Mar     | kus Stricker   |       |                       |        |                |  |
| 11                                      | Other inf   | ormation              |                   |                |       |                       |        |                |  |
|   | -   |                       |                   |                |       |                       |        |                |  |

| NON | NON-TECHNICAL ELECTIVE MODULE - RUB SOFT SKILLS/LANGUAGE COURSE |                        |                  |                |       |                       |        |                  |  |  |  |
|-----|---|------------------------|------------------|----------------|-------|-----------------------|--------|------------------|--|--|--|
| Mod | ule code  | Student                | Credits          | Semeste        | r     | Frequency             |        | Duration         |  |  |  |
|     | 10  | workload               | 3 ECTS           | 2nd            |       | summer term           |        | 1 semester       |  |  |  |
|     |   | 120 hours              |                  |                |       | free choice of        |        |                  |  |  |  |
|     |   |                        |                  |                |       | available module      | es     |                  |  |  |  |
| 1   | Types of o  | courses:               | Contact he       | ours           | Ind   | lependent study       | Cla    | ss size          |  |  |  |
|     | lecture ar  | nd class               | 45 hrs           |                | 75    | hours                 |        |                  |  |  |  |
| 2   | Learning  | outcomes               |                  |                |       |                       |        |                  |  |  |  |
|     | Students  | broaden their kno      | wledge base, sl  | kills, or metl | nod s | spectrum according    | to th  | eir personal in- |  |  |  |
|     | terests.  |                        |                  |                |       |                       |        |                  |  |  |  |
| 3   | Subject a   | ims                    |                  |                |       |                       |        |                  |  |  |  |
|     | • I   | Develop knowledge      | and skills in fi | elds beyond    | eng   | ineering and scienc   | e      |                  |  |  |  |
|     | • (   | Gain and develop k     | nowledge in no   | on-technical   | subj  | ects, related to mate | erials | engineering,     |  |  |  |
|     | like business administration according to own interests         |                        |                  |                |       |                       |        |                  |  |  |  |
|     | • [   | Develop and practic    | e communicat     | ion skills     |       |                       |        |                  |  |  |  |
| 4   | Teaching  | methods                |                  |                |       |                       |        |                  |  |  |  |
|     | see specif  | ic module descript     | ions             |                |       |                       |        |                  |  |  |  |
| 5   | Prerequis   | ites for participation | on               |                |       |                       |        |                  |  |  |  |
|     | none  |                        |                  |                |       |                       |        |                  |  |  |  |
| 6   | Assessme  | ent methods            |                  |                |       |                       |        |                  |  |  |  |
|     | written or  | oral examination       | as given in spe  | cific module   | des   | cription              |        |                  |  |  |  |
| 7   | Prerequis   | ites for the assignr   | nent of credit p | points         |       |                       |        |                  |  |  |  |
|     | passing th  | ne examination         |                  |                |       |                       |        |                  |  |  |  |
| 8   | This mod  | ule is used in the f   | ollowing degre   | e programn     | ies a | s well                |        |                  |  |  |  |
|     | none  |                        |                  |                |       |                       |        |                  |  |  |  |
| 9   | Impact of   | grade on total grad    | de               |                |       |                       |        |                  |  |  |  |
|     |   |                        |                  |                |       |                       |        |                  |  |  |  |
| 10  | Responsi  | bility for module      |                  |                |       |                       |        |                  |  |  |  |
| 11  | see specif  | ic module descript     | 1011             |                |       |                       |        |                  |  |  |  |
| 11  | Other inf   | ormation               |                  |                |       |                       |        |                  |  |  |  |
|     | -   |                        |                  |                |       |                       |        |                  |  |  |  |



| MATERIALS MODELLING LAB |                  |                        |                  |                |                  |                      |               |             |  |  |
|-------------------------|------------------|------------------------|------------------|----------------|------------------|----------------------|---------------|-------------|--|--|
| Mod                     | lule code        | Student work-          | Credits          | Semester       | r                | Frequency            | D             | uration     |  |  |
|                         | 11               | load                   | 6 ECTS           | 1st            |                  | Winter term          | 1 s           | emester     |  |  |
|                         |                  | 180 hours              |                  |                |                  |                      |               |             |  |  |
| 1                       | Types of o       | courses                | Contact          | hours          | Ind              | lependent study      | Class size    |             |  |  |
|                         | class            |                        | 45 hrs (3        | SWS)           | 135              | hours                | 30 student    | IS          |  |  |
| 2                       | T                |                        |                  |                |                  |                      |               |             |  |  |
| Z                       | Learning         | outcomes               | n matoriala r    | alated comp    | itor a           | simulations on diff  | oront time    | nd longth   |  |  |
|                         | scales Th        | are able to perior     | alvze the sin    | vulation resul | ller s<br>Ite ar | ad summarize and     | discuss the   | m in short  |  |  |
|                         | written re       | ports They learn       | self-organiza    | tion and tim   | e ma             | in summarize and     | ning perfor   | ming and    |  |  |
|                         | evaluating       | simulations along      | the standard     | ls of good res | earc             | h practice.          |               | iiiiig uiiu |  |  |
| 3                       | Subject ai       | ims                    | )                | 0              |                  | -1                   |               |             |  |  |
|                         | The follow       | ving methods will l    | be introduced    | l and applied  | for c            | omputer simulatior   | ns of materia | al behavior |  |  |
|                         | at various       | length and time so     | ales:            |                |                  | _                    |               |             |  |  |
|                         | • E              | Electronic structure   | calculations     | (Density Fun   | ctior            | nal Theory)          |               |             |  |  |
|                         | • N              | Aolecular Dynamic      | s                |                |                  |                      |               |             |  |  |
|                         | • F              | hasefield              |                  |                |                  |                      |               |             |  |  |
|                         | • (              | Calculation of Phase   | e Diagrams (     | CalPhaD)       |                  |                      |               |             |  |  |
|                         | • N              | Aicromechanical si     | mulations wi     | th the Finite  | Elen             | ient Method          |               |             |  |  |
|                         | • A              | Artificial Intelligenc | e and machi      | ne learning    |                  |                      |               |             |  |  |
| 4                       | Teaching methods |                        |                  |                |                  |                      |               |             |  |  |
| 5                       | Class With       | ites for participatio  | omputer exp      | eriments) as i | eam              | work in teams of 2-  | 3 students    |             |  |  |
| J                       | None             | nes for participatio   | 11               |                |                  |                      |               |             |  |  |
| 6                       | Assessme         | ent methods            |                  |                |                  |                      |               |             |  |  |
|                         | Oral exan        | n (20 minutes)         |                  |                |                  |                      |               |             |  |  |
|                         | Group wo         | ork for each experir   | nent: entranc    | e exam (5-10   | min              | utes), written repor | t (3-5 pages) | and oral    |  |  |
| 7                       | discussion       | n of results (5-10 m   | inutes) for each | ach team       |                  |                      |               |             |  |  |
| /                       | Prerequis        | f oral exam and acc    | conted writter   | reports of al  | 1 ovr            | eriments: up to two  | ovnorimon     | te can be   |  |  |
|                         | repeated         |                        | epieu wiittei    | i reports of a | і слр            | eriments, up to two  | скрепшен      |             |  |  |
| 8                       | This mod         | ule is used in the f   | ollowing deg     | ree programn   | nes a            | s well               |               |             |  |  |
|                         | none             |                        |                  | F - 8          |                  |                      |               |             |  |  |
| 9                       | Impact of        | grade on total grad    | le               |                |                  |                      |               |             |  |  |
|                         | 6/117            | 0 0                    |                  |                |                  |                      |               |             |  |  |
| 10                      | Responsi         | bility for module      |                  |                |                  |                      |               |             |  |  |
|                         | Prof. Dr.        | Alexander Hartmai      | er, Dr. Oleg     | Shchyglo       |                  |                      |               |             |  |  |
| 11                      | Other info       | ormation               |                  | .1 . 1 1       | 1                |                      | 11 - 1        |             |  |  |
|                         | A lecture        | script, including in   | ion locture h    | o the individu | al e             | xperiments is provi  | aed. Each e   | xperiment   |  |  |
|                         | consists o       | f the results a surrit | ton report on    | d the discuss  | sor, a           | all entry exam, the  | computer s    | rinulation, |  |  |
|                         | anaiysis o       | i me results, a writ   | ten report an    | u the discuss  |                  | n me report with th  | e supervisoi  | •           |  |  |



| RESEARCH PROJECT |   |                       |                  |               |        |                      |        |                 |  |  |
|------------------|---|-----------------------|------------------|---------------|--------|----------------------|--------|-----------------|--|--|
| Mod              | lule code   | Student               | Credits          | Semeste       | er     | Frequency            |        | Duration        |  |  |
|                  | 12  | workload              | 6 ECTS           | 3rd           |        | continuous offers    | of     | 1 semester      |  |  |
|                  |   | 180 hours             |                  |               |        | topics               |        |                 |  |  |
|                  |   | (4 months)            |                  |               |        |                      |        |                 |  |  |
| 1                | Types of o  | courses:              | Contact he       | ours          | Inc    | lependent study      | Cla    | ss size         |  |  |
|                  | practical v   | work                  | 20 hrs           |               | 160    | ) hours              | 1-3    | students        |  |  |
| 2                | Learning outcomes   |                       |                  |               |        |                      |        |                 |  |  |
|                  | The students can structure a complex research task into sub-tasks and work packages. They develop |                       |                  |               |        |                      |        |                 |  |  |
|                  | individual  | l problem solution    | strategies to ta | ckle differe  | nt ta  | sks by applying scie | ntific | c methods. Stu- |  |  |
|                  | dents are   | able to report and    | present scienti  | fic projects. |        |                      |        |                 |  |  |
| 3                | Subject ai  | ms                    |                  |               |        |                      |        |                 |  |  |
|                  | Treatmen  | t of a scientific sub | ject in a given  | time          |        |                      |        |                 |  |  |
|                  | Scientific  | solution for a give   | n practical prol | olem          |        |                      |        |                 |  |  |
|                  | Application of learned techniques from previous modules   |                       |                  |               |        |                      |        |                 |  |  |
|                  | leamwor   | K                     | 1.               |               |        |                      |        |                 |  |  |
|                  | Written p   | resentation of the i  | results          |               |        |                      |        |                 |  |  |
| 4                | Teaching  | methods               | به مابا ممانه م  |               |        | :                    |        |                 |  |  |
|                  | continuot   | as contact periods t  | o advice the st  | udent, prese  | entat  | ion of progress duri | ng g   | roup seminars   |  |  |
| 5                | Broroquis   | itos for participatio | n                |               |        |                      |        |                 |  |  |
| 2                | successfu   | l completion of all   | ompulsory m      | odules of fir | ret ai | nd second semester   |        |                 |  |  |
| 6                | Assessme  | nt methods            | compulsory m     | oduics of m   | sta    | iu seconu semester   |        |                 |  |  |
| Ŭ                | written re  | port (20 to 50 page   | S)               |               |        |                      |        |                 |  |  |
| 7                | Prerequis   | ites for the assignr  | nent of credit i | points        |        |                      |        |                 |  |  |
| -                | positively  | evaluated written     | report           |               |        |                      |        |                 |  |  |
| 8                | This mod  | ule is used in the f  | ollowing degre   | e programn    | nes a  | s well               |        |                 |  |  |
|                  | none  |                       | 0 0              | 1 0           |        |                      |        |                 |  |  |
| 9                | Impact of   | grade on total grad   | le               |               |        |                      |        |                 |  |  |
|                  | 6/117   |                       |                  |               |        |                      |        |                 |  |  |
| 10               | Responsi  | bility for module     |                  |               |        |                      |        |                 |  |  |
|                  | all lecture   | rs of the Master co   | urse             |               |        |                      |        |                 |  |  |
| 11               | Other info  | ormation              |                  |               |        |                      |        |                 |  |  |
|                  | -   |                       |                  |               |        |                      |        |                 |  |  |





| MAS | TER TH  | ESIS   |                  |               |                           |                      |  |  |  |
|-----|---|--|------------------|---------------|---------------------------|----------------------|--|--|--|
| Mod | lule code   | Student                                      | Credits          | Semester      | Frequency                 | Duration             |  |  |  |
|     | 13  | workload                                     | 30 ECTS          | 4th           | continuous offers         | s of 1 semester      |  |  |  |
|     | -   | 900 hours                                    |                  |               | topics                    |                      |  |  |  |
| 1   | Types of o  | courses:                                     | Contact he       | ours          | Independent study         | Class size           |  |  |  |
|     | practical v   | work   | 100 hrs          |               | 800 hours                 | 1 student            |  |  |  |
| 2   | 2 Learning outcomes<br>After successful completion of the master thesis students are in a position to independently process<br>research tasks by applying scientific methods within a predefined period of time. In particular, they<br>are able to independently plan, organize, develop, operate and present research tasks from the field<br>of materials science. They develop advanced problem solution strategies to tackle different tasks by<br>applying the theoretical knowledge gained in the Master course. Students are able to report and pre-<br>sent the progress scientific projects, to summarize their results in an oral presentation, and to write |  |                  |               |                           |                      |  |  |  |
|     | a scientifi   | c project documen                            | tation.          |               | researce in an oral pres  |                      |  |  |  |
| 3   | Subject aims         Independent scientific project         Application of learned techniques from previous modules         Independent identification and solution of scientific problems         Literature survey         Written and oral presentation of the results   |  |                  |               |                           |                      |  |  |  |
| 4   | Teaching<br>continuou<br>discussion   | <b>methods</b><br>us contact to advice<br>ns | e the student, p | resentation c | f progress during grou    | ıp seminars and      |  |  |  |
| 5   | Prerequis   | ites for participation                       | on               |               |                           |                      |  |  |  |
|     | successfu   | l completion of pro                          | oject work (mo   | dule 12) and  | a total of at least 80 EC | CTS from all modules |  |  |  |
| 6   | Assessme  | ent methods                                  | N 000/           | 1 1           |                           |                      |  |  |  |
| 7   | written th  | iesis (40 to 150 pag                         | es) 80%, asses   | sed oral pres | entation 20%              |                      |  |  |  |
| /   | prerequis   | ovaluated thegin                             | nent of credit j | points        |                           |                      |  |  |  |
| 8   | This mod  | ule is used in the f                         | following degre  | e programm    | es as well                |                      |  |  |  |
| Ū   | none  | uie is used in the i                         | onowing degre    | e programmi   |                           |                      |  |  |  |
| 9   | Impact of   | grade on total grad                          | de               |               |                           |                      |  |  |  |
|     | 30/117  | 0 0  |                  |               |                           |                      |  |  |  |
| 10  | Responsi  | bility for module                            |                  |               |                           |                      |  |  |  |
|     | all lecture   | ers of the Master co                         | ourse            |               |                           |                      |  |  |  |
| 11  | Other inf   | ormation                                     |                  |               |                           |                      |  |  |  |
|     | -   |  |                  |               |                           |                      |  |  |  |



