Module title: Materials Design
Abbreviation: MD
Study program: Mechanical engineering Bachelor
Term: 6MB 7MB
Turnus: Annual rhythm
Language: English
Responsible: Prof.-Dr. T. Markus
Lecturer: Prof.-Dr. T. Markus
Course type: Elective
SWS: 4
Credits: 5
Requirements: Knowledge in Thermodynamics and Materials Science, Mathematics, Interest in developing algorithms

Education objective:
The availability of computer algorithms supports engineers to simulate materials properties for specific demands. Therewith experimental effort to develop application oriented materials can be significantly reduced. Combining simulation- and experimental results is the basis for modern and advanced materials development.

Upon completion of the course, students will have gained basic knowledge about:
1. Methods of computer based materials design,
2. Development of materials databases using available materials data as well as estimations,
3. Simulation of materials properties and their variation with temperature, time, pressure, respectively,

Work load:

<table>
<thead>
<tr>
<th></th>
<th>Hours</th>
<th>Self-study</th>
<th>Credits</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWS</td>
<td>Σ hrs. during term</td>
<td>hrs.</td>
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<tr>
<td>Lecture:</td>
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<td>30</td>
<td>15</td>
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<td>Practice:</td>
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<tr>
<td>Laboratory:</td>
<td>2</td>
<td>30</td>
<td>35</td>
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<tr>
<td>Exam preparation:</td>
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<tr>
<td><strong>Total</strong></td>
<td>4</td>
<td>60</td>
<td>90</td>
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Course Topics:

1. **Overview upon Materials Design Methods**
   - From basics towards applications
2. **Fundamentals**
   - what is the aim of materials design processes
   - Materials science
   - Thermodynamics
   - Mathematics
   - Which materials properties are needed?
3. **Structure of a materials base**
4. **Algorithms**
   - Description of equilibrium states
   - Constitutional- and phase diagrams
   - Calculation of reaction paths and phase changes
   - Kinetics and diffusion
5. **Software tools**
6. **Application and Case studies**
   - Various problem oriented approaches

Teaching method: Lecture and PC laboratory
Program: Lecture, group work, term paper
| achievement: |  |
| examination method | Project work or written examination 90 minutes or oral examination 30 min (announced at start of term). |
- Additional technical literature on special topics  
- Tutorial and Skript |
| update: | 05.07.2017 |