1. Annotation

Course Description

The course provides an overview of modern atomistic computer simulations used to model, understand, and predict properties of realistic materials. The emphasis is on practical techniques, algorithms and programs to bridge theory and applications, from the discovery of materials to their use in real-world technologies. This introductory course is intended for both theoreticians and experimentalists in modern Materials Science at academic level ranging from MSc students to PhD students and postdocs.

Course Prerequisites / Recommendations

The course relies on basic knowledge of theoretical physics or chemistry including quantum mechanics and statistical physics at undergraduate level. Ideally it should follow an introductory course in Materials Science.

2. Structure and Content
### Course Academic Level

Master-level course suitable for PhD students

### Number of ECTS credits

6

<table>
<thead>
<tr>
<th>Topic</th>
<th>Summary of Topic</th>
<th>Lectures (# of hours)</th>
<th>Seminars (# of hours)</th>
<th>Labs (# of hours)</th>
</tr>
</thead>
</table>
| Computational Quantum Chemistry | 1. Introduction. Basics of quantum chemistry  
2. Hartree-Fock and post-HF  
3. Density functional theory  
4. Excited states and dynamics  
5. Computational chemistry of molecules  
6. Computational chemistry of crystals | 12                    | 15                    | 0                  |
| Materials Modeling            | 7. Tight binding and semiempirical methods  
8. Classical molecular mechanics  
9. Classical molecular dynamics. Nonadiabatic dynamics  
10. Defects in solids  
11. Chemical reactions  
12. Modeling of organic semiconductors  
13. Guest lecture | 14                    | 13                    | 0                  |
| Final project                 | Final project                                                                   | 0                     | 15                    | 0                  |

### 3. Assignments

**Assignment Type**

**Homework**

Take a molecule with at least 10 atoms. Using semiempirical Hamiltonian of your choice:
Optimize ground state geometry. Check its stability. Determine if it is the global minimum.
Plot frontier orbitals (HOMO-LUMO). Calculate the energy gap. Calculate localized molecular orbitals and explain electronic structure and geometry. Optimize geometry of the lowest energy triplet state (or cation, or anion, if more appropriate for your project). Calculate the relative energy of the triplet state. Plot unpaired molecular orbitals. Explain changes in electronic structure and geometry relative to the singlet state. The solution should be prepared in the form of a written report supplemented by the required technical les: xyz-geometries, mgf-orbitals, program run log-les, gures not inserted into the report etc. Be prepared to give a 5 min presentation of everything that you consider nontrivial in your work.
**Team Project**

Formulate your own project within the above defined topic or do one of the following projects:

1. Explain the structural and electronic properties of linear \( \text{C}_n\text{H}_n+2 \) (polyacetylene and its oligomers) and cyclic \( \text{C}_n\text{H}_n \) (annulenes) alkenes (use a semiempirical approach).
2. Illustrate pseudo Jahn-Teller effect in AX3 molecules.
3. Explore shapes of elemental small clusters.
4. Explain bonding in SF6 molecule.
5. Illustrate lone-pair concept.
6. Illustrate hybridization of orbitals.
7. Where is the boundary between covalent and ionic bonding?
8. Illustrate secondary bonding.
9. Explain and illustrate duodecet rule.
10. Solve 2c2e model.
11. Solve 4c4e model.
12. Solve 6c6e benzene model.

**Format**

- Conference-style presentation: 20-min, 15-30 slides
- Article-style report: 5-10 pages of original text + unlimited number of figures and tables + at least 10-20 references

**How to choose the final project**

- Your own choice, e.g. your current or future research
- Follow-up of a team project
- Follow-up of a research paper
- Review a research paper
- Prepare a short lecture and recitation
- Solve a complex problem from this set (marked by (60) and above)

If your final project is your mainstream research project,

- Start it as soon as possible
- Replace team projects by independent parts of your research project (relevant to the announced topic)
- In Homework Labs use systems from your research project
- Materials currently modeled at CEE CREI
  - Inorganic cathodes for metal-ion batteries (Dmitry Aksenov - Artem Abakumov)
  - Organic cathodes for metal-ion batteries (Andriy Zhugayevych - Pavel Troshin)
  - Ion transport through membranes in redox flow batteries (Andriy Zhugayevych - Keith Stevenson)
  - Molecular crystals for field effect transistors (Andriy Zhugayevych - Pavel Troshin)
  - Conjugated polymers for solar cells (Olga Mazaleva - Pavel Troshin)
  - Perovskites for solar cells (Sergei Tretiak - Pavel Troshin)
  - Structure of semicrystalline conjugated polymers (Andriy Zhugayevych - Pavel Troshin)

**4. Grading**

<table>
<thead>
<tr>
<th>Type of Assessment</th>
<th>Graded</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grade Structure</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Activity Type</th>
<th>Activity weight, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Homework Assignments</td>
<td>33</td>
</tr>
<tr>
<td>Final Project</td>
<td>33</td>
</tr>
<tr>
<td>Projects</td>
<td>20</td>
</tr>
<tr>
<td>Class participation</td>
<td>14</td>
</tr>
</tbody>
</table>
5. Basic Information

Course Stream: Science, Technology and Engineering (STE)
Course Term (in context of Academic Year): Term 2
Course Delivery Frequency: Every year

Students of Which Programs do You Recommend to Consider this Course as an Elective?

<table>
<thead>
<tr>
<th>Masters Programs</th>
<th>PhD Programs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Materials Science</td>
<td>Computational and Data Science and Engineering</td>
</tr>
<tr>
<td>Photonics and Quantum Materials</td>
<td>Materials Science and Engineering</td>
</tr>
<tr>
<td></td>
<td>Physics</td>
</tr>
<tr>
<td></td>
<td>Materials Science and Engineering Physics</td>
</tr>
</tbody>
</table>

Course Tags: Physics, Engineering, Chemistry

6. Textbooks and Internet Resources

<table>
<thead>
<tr>
<th>Required Textbooks</th>
<th>ISBN-13 (or ISBN-10)</th>
</tr>
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</table>
### 7. Facilities

#### Equipment

<table>
<thead>
<tr>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room equipped with audio, video, WiFi</td>
</tr>
<tr>
<td>Virtual Machine on Pardus cluster</td>
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</tbody>
</table>

#### Software

<table>
<thead>
<tr>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>MOPAC, Gaussian, VASP, LAMMPS, Jmol, Python, Maple</td>
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</tbody>
</table>

**Labs for Education**

CEE CREI Computational Lab

### 8. Learning Outcomes

#### Knowledge

Fundamentals of the modern computational methods for molecular, nano- and meso-scale materials modeling that cover a wide time and length scales.

#### Skill

Apply fundamental knowledge about materials modeling via computer simulations including terminology, key concepts, methods and topics of study
Experience

Use commercial and free/copyleft (GNU) modeling and visualization software for materials science studies, including computations on HPC clusters

9. Assessment Criteria

Input or Upload Example(s) of Assignment 1:

<table>
<thead>
<tr>
<th>Select Assignment 1 Type</th>
<th>Homework Assignments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input Example(s) of Assignment 1 (preferable)</td>
<td><a href="http://zhugayevych.me/edu/CC/Homework2.pdf">http://zhugayevych.me/edu/CC/Homework2.pdf</a></td>
</tr>
</tbody>
</table>

Assessment Criteria for Assignment 1

Identical homework solutions are not counted. Additional homeworks may be taken to replace the worst grades.

Input or Upload Example(s) of Assignment 2:

<table>
<thead>
<tr>
<th>Select Assignment 2 Type</th>
<th>Team Project</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input Example(s) of Assignment 2 (preferable)</td>
<td><a href="http://zhugayevych.me/edu/CC/Project1.pdf">http://zhugayevych.me/edu/CC/Project1.pdf</a></td>
</tr>
</tbody>
</table>

Assessment Criteria for Assignment 2

Projects are assessed as follows:
40% – written report (75% content, 25% presentation)
40% – oral presentation (50% content, 25% presentation, 25% discussion)
20% – discussion of other projects

Input or Upload Example(s) of Assignment 3:

<table>
<thead>
<tr>
<th>Select Assignment 3 Type</th>
<th>Final Project</th>
</tr>
</thead>
<tbody>
<tr>
<td>Input Example(s) of Assignment 3 (preferable)</td>
<td><a href="http://zhugayevych.me/edu/Materials/FinalProject.htm">http://zhugayevych.me/edu/Materials/FinalProject.htm</a></td>
</tr>
</tbody>
</table>

Actual projects in 2015:
- NHO system
- polyaniline
- confined water

Assessment Criteria for Assignment 3

Projects are assessed as follows:
40% – written report (75% content, 25% presentation)
40% – oral presentation (50% content, 25% presentation, 25% discussion)
20% – discussion of other projects
<table>
<thead>
<tr>
<th>Input or Upload Example(s) of Assignment 4:</th>
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<tbody>
<tr>
<td>Input or Upload Example(s) of Assignment 5:</td>
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<td>--------------------------------------------</td>
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</table>

10. Additional Notes

<table>
<thead>
<tr>
<th>Free Style Comments (if any)</th>
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</thead>
<tbody>
<tr>
<td>Please see the course website for syllabus and other information: <a href="http://zhugayevych.me/edu/CC/index.htm">http://zhugayevych.me/edu/CC/index.htm</a></td>
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