MSE 7193.02 Advanced Atomic Scale Computational Materials Modeling

Syllabus prepared on February 27, 2019, by the instructor:

Maryam Ghazisaeidi, Assistant Professor; ghazisaeidi.1@osu.edu
The Ohio State University
Department of Materials Science and Engineering
Office hours: TBD

GENERAL INFORMATION:

**Lecture time:** 14wk; time: TBD; location: TBD.

**Purpose:** A project-based in-depth exploration of state-of-the-art computational methods in materials research with emphasis on the atomic scale.

**Level & credit:** TWO graduate credit, MSE 7193.02 class number XXX

**Prerequisites:** MSE 6756.02 (Computational Materials Modeling – Atomistic Methods) or 6756 (Computational Materials Modeling) with excellent grade, or permission by instructor.

**Course material:** No required text book. All class notes, software, and reading will be available on carmen.osu.edu.

CLASS FORMAT:

Combination of lectures and active learning student projects. Examples of topics include: Fundamentals of density functional theory, Ab initio Thermodynamics, Electronic structure, Magnetic properties and Beyond standard DFT.

COURSE POLICIES:

1. **Grading policy:**
   *Graded course. Numerical scores:* The total weight of the course is approximately divided as follows:
   Homework / lab 50%
   Active learning 50%

**Active learning activities:** In consultation with the instructor, each student will either alone or in a team, depending on the number of participants, prepare material for a specific sub topic of the classes, introduce it to their peers, and evaluate the results.
SOFTWARE

- The course will focus on electronic structure methods and especially DFT. We will mostly use VASP, something else if necessary.
- Time-consuming calculations will be run on the supercomputers of the Ohio Supercomputer Center (you will be provided with an account at OSC).

COURSE EVALUATION

Students are requested to evaluate the course during the last weeks of the semester. Further instructions on how to complete the evaluation will be provided by that time. As part of the course evaluation, students are requested to present any and all constructive criticism they believe would enhance this course in future offerings.

DISABILITY SERVICES

The Office for Disability Services coordinates physical and academic support services for any student who has the need because of a permanent or temporary disability. Individuals eligible for services include, but are not limited to, those with mobility, hearing, visual, speech, or learning disabilities. Services are available on a self-referral basis. Successful accommodation often requires advance planning. Students are encouraged to make early contact with The Office of Disability services to identify their needs and ensure that services will be available in an effective and timely manner. The Office for Disability Services is located at 150 Pomerene Hall, 1760 Neil Avenue, telephone # 292-3307.

ACADEMIC INTEGRITY, ACADEMIC MISCONDUCT

Academic misconduct may be found in any action that tends to distort the accurate assessment of any student’s individual accomplishments that are evaluated for the purpose of grading or conferring academic credit. Note that a student may be guilty of academic misconduct, for example, by cheating, collaborating, plagiarizing, or by allowing another student to cheat, collaborate, or plagiarize. Note also that the distortion applies, for example, to exams, homework assignments, and laboratory work. To the extent that any class activity (for example: attendance or participation) is used for evaluation for the purpose of grading or conferring academic credit, falsifying or distorting such activity, or permitting another student to falsify or distort such activity, represents academic misconduct.

For more, and for additional resources, see https://mse.osu.edu/academic-integrity-disability-accommodation-statements

DIVERSITY AND INCLUSION

The Ohio State University and Department of Materials Science and Engineering affirm the importance and value of diversity in the student body. We are committed to maintaining a community that recognizes and values the inherent worth and dignity of every person; fosters sensitivity, understanding, and mutual respect among all members of our community; and encourages each individual to strive to reach their own potential. Discrimination against any individual based upon protected status, which is defined as age, disability, gender identity or expression, national origin, race, ethnicity, religion, sex, sexual orientation, or veteran status, is prohibited.