

## MSE 7193.02 DFT and Interatomic Potentials

Syllabus prepared on November 9, 2021, by current instructor:

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Department of Materials Science and Engineering

Office hours: TBD

### GENERAL INFORMATION:

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

**Purpose:** A project-based in-depth exploration of methods and implementations to develop interatomic potentials from density-functional theory data.

**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), plus at least one specialty DFT class taught by Dr. Ghazisaeidi or Dr. Windl.

**Course material:** No required text book. All class notes, software, and reading will be available on [carmen.osu.edu](https://carmen.osu.edu).

### COURSE POLICIES:

#### 1. Topics:

This course will explore common interatomic potentials types (including machine learning potentials) and fitting tools and develop practical proficiency to fit and develop new potentials based on DFT-calculated input data.

#### 2. Grading policy:

*Graded course. Numerical scores:* The total weight of the course is *approximately* divided as follows:

Homework / lab 50%

Final project 50%

3. **Homework/lab:** Each class will be dedicated to a specific modeling task and/or potential type. Students will perform computations as assignments and report their results at the beginning of the following class.

4. **Research design project:** Students will develop individually or in teams new interatomic potentials for systems related to their research, ideally with quantified uncertainties.

## **SOFTWARE**

- The course will focus on electronic structure methods and especially DFT for input data. We will mostly use VASP, something else if necessary.
- The course will use LAMMPS as deployment and development platform for the interatomic potentials (or other if agreed upon)
- Time-consuming calculations will be run on the supercomputers of the Ohio Supercomputer Center (you will be provided with a class 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>