MSE 8193: Atomistic Modeling of Transport Phenomena

Syllabus prepared on February 20, 2019 by instructor:

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PURPOSE: Develop an understanding of atomistic modeling of transport processes in materials – diffusion, solid-state reactions, heat transport, electron transport through a practical hands-on introduction on realistic examples.

LEVEL: G. U by permission of instructor.

LECTURE TIME: W 2:20-4:10 pm (Smith 5097 computer lab)
full-semester course
2 Cr. Hrs in one 110-minute session;
offered in “Spring”.

PREREQUISITES:
- Successful completion of MSE 6756.02 (Introduction to Atomistic Modeling), or permission by instructor.

COURSE MATERIAL:
- No required textbook. All class notes, software, and reading assignments will be available on carmen.osu.edu.

LECTURE TOPICS:
- Harmonic transition state theory – Arrhenius equation, energy barriers, activation energies, and prefactors.
  - Elastic band methods
  - Dimer method
  - Vineyard theory
  - Kinetic parameters vs. reaction rates
  - Defining parameters for rate-theory based modelling
- Transition state theory vs. MD modelling of kinetic processes
  - Einstein diffusion coefficients
  - Correlation functions and Green-Kubo diffusion coefficients
- Heat transport
  - Phonon based
- Linearized Boltzmann transport and phonon anharmonicity
- Non-equilibrium molecular dynamics
- Correlation functions and Green Kubo theory
  - Electron based
    - Wiedmann-Franz-Lorenz law and look at electron conduction
- Electron transport
  - Effective masses and electron mobility
  - From band structures to Boltzmann transport theory

**GRADING PLAN:**
- Weekly lab assignments (75%)
- Final design project as final exam (20%)
- Attendance and participation, 5%.

**COURSE EVALUATION:**
Students are requested to evaluate the course during the last weeks of the quarter. 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.

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