Atomic Scale Simulations

May 15 – May 26, 2017

Universidade Federal do ABC

What To Expect:

This 2-week intensive course aims at senior undergraduate, graduate, and postdoctoral scholars. Attendees will be introduced to:

- the theoretical background of powerful modern molecular dynamics and Monte-Carlo schemes,
- predictive quantum-mechanical approaches such as density functional theory,
- hands-on experience with Python coding, visualization, and running own simulations using freely available open-source software packages.

Morning lectures provide theoretical background and afternoons are for hands-on practice and implementation in computer labs. This combination conveys good understanding of all theoretical approaches. Attendees will develop their own ideas for a toy problem, implement small parts of code if necessary, run simulations, and write a short report on results and obstacles encountered.

Course Description:

This class covers computational techniques for microscopic systems ranging from a few up to millions of atoms. Molecular dynamics provides exciting insight into the dynamic aspect of thermodynamic phase-space averages. Important concepts, such as potential-energy surfaces, classical potentials, and their quantum-mechanical foundation will be outlined. Connections to accurate, computationally expensive methods, e.g. those based on density functional theory will be pointed out. Furthermore, this class covers probabilistic Monte-Carlo techniques, that differ conceptually: The idea of probabilistic integration, Markov-Chain approaches, and Metropolis Monte-Carlo will be presented. Examples for practical applications of the different techniques are discussed throughout.

Interested? Please register!

Go to this web form to sign up and to provide us with some information on your background, which helps us to plan this class: https://goo.gl/forms/furolq2YpBwS11S93

Questions? Feel free to contact us anytime!

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APS physics

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