future ocean
KIEL MARINE SCIENCES

Workshop on

Molecular Dynamics - a computational tool for the molecular understanding of nature

Prof. Dr. Bernd Hartke & Dr. Evangelos Voyiatzis
(Institute of Physical Chemistry, Kiel University)

13 November 2017

In this course you get a concise introduction to Molecular Dynamics (MD) simulations. MD is an emerging computational technique in marine science that provides a link between the microscopic structure of a system and its macroscopic properties. It is particularly useful for studying systems at small length scales with molecular resolution. For example, questions such as "What determines molecular transport across the water-air interface?", "What are the time-scales and dynamics for competitive adsorption of organics at bubble surfaces?", and many more can be addressed.

You are invited to bring and discuss with the trainers your ideas on how to apply this technique for your own research.
The course targets both doctoral candidates as well as postdoctoral researchers from all disciplines; no prior knowledge of the technique is required.
The general introduction lecture is also open to senior researchers who are looking for a quick overview of the MD technique.

Open to Everyone:
09:00 – 10:30 h **Introductory Overview Lecture**
10:45 – 12:00 h Theoretical & Practical Background

Registration required for:
13:00 – 16:15 h Hands-On Molecular Dynamics
16:15 – 17:00 h Round Table Discussion

Course Content:
- General introduction into the concept of Molecular Dynamics
- Introduction to some theoretical aspects and practical pitfalls
- Hands-on examples using open source programs LAMMPS and VMD (comparison of different models for water, structure and dynamical properties of aqueous solutions, mechanical properties of silica, etc.)

Venue: *Leibnizstr. 1, room 105*
Usually, child care can be provided – please get in touch with us as soon as possible.

Please register online at
www.futureocean.org/isos

C|A|U Kiel University Christian-Albrechts-Universität zu Kiel
ifw
muthesius kunsthochschule
GEOMAR