

2014 SYMPOSIUM ON MOLECULAR DYNAMICS (MD) FOR ENGINEERING AND SCIENCE

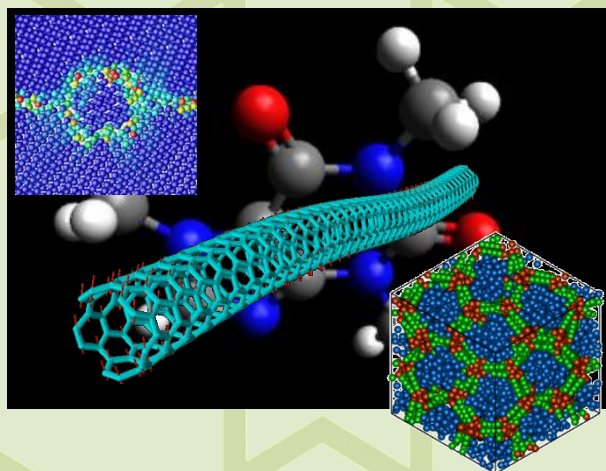
AUDITORIUM EDIFICIO SAN AGUSTÍN
SCHOOL OF ENGINEERING, PONTIFICIA UNIVERSIDAD CATÓLICA DE CHILE
VICUÑA MACKENNA 4860, MACUL, SANTIAGO

Organizers: Ingeniería-PUC and Ciencias-UCh

Symposium, December 9th; Tutorial, December 10th

SYMPOSIUM CHARACTERISTICS

This symposium will take place at Campus San Joaquín, Pontificia Universidad Católica de Chile on December 9th and 10th, 2014. This Symposium is directed to graduate students, researchers and practitioners of the MD methods for Engineering and Science. This Symposium will be organized around talks by invited national and international speakers. A tutorial on the basic of MD will be held at Campus San Joaquin on Wednesday, December 10th between 14:00 and 18:00 hrs.



Symposium Agenda

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| 14:00-14:15 | Opening words: purpose and objectives |
| 14:15-14:45 | Atomistic simulation copper-based nanowires under tensile stress and compression , Gonzalo Gutiérrez, Facultad de Ciencias, Universidad de Chile |
| 14:45-15:15 | Fitting of interatomic potentials without forces: a parallel particle swarm optimization algorithm , Sergio Davis, Facultad de Ciencias, Universidad de Chile |
| 15:15-15:45 | Innovative Nano Materials for Unconventional Thermal Transport Control , Tengfei Luo, University of Notre Dame, USA |
| 15:45-16:00 | Coffee break |
| 16:00-16:30 | Ab Initio Free Energy Calculations of the Solubility of Silica in Metallic Hydrogen , Felipe Gonzalez, Facultad de Ciencias, Universidad de Chile |
| 16:30-17:00 | Electronic, dielectric, and optical properties of the B phase of niobium pentoxide and tantalum pentoxide by first-principles calculations , Camilo Valencia, Instituto Tecnológico Metropolitano, Medellín, Colombia |
| 17:00-17:30 | Directional Solvent for Membrane-Free and Low-Temperature Water Desalination , Tengfei Luo, University of Notre Dame, USA |
| 17:30-18:00 | Structure and Dynamic Studies for a Binary System of Menadione in Supercritical CO₂ , Andrea Reveco, Escuela de Ingeniería, PUC |
| 18:00-18:30 | Summary, comment and remarks |

Invited Speaker



Tengfei Luo, Ph.D.
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