Università di Cagliari

DIPARTIMENTO DI SCIENZE CHIMICHE E GEOLOGICHE
ANNUNCIO DI SEMINARI

Nell'ambito del **Programma "Visiting Professor 2014/2015" finanziato dalla Regione Sardegna,** il Visiting **Professor Aatto Laaksonen**, del Material and Environmental Chemistry Dept. della Stockholm University e dello Scilife Lab del Karolinska Institute, terra' una serie di seminari riguardanti diversi aspetti delle simulazioni e della modellistica molecolare moderna.

Nei seminari iniziali verra' discusso lo stato dell'arte relativamente ai metodi e ai modelli correntemente utilizzati nella chimica computazionale, partendo da schemi di simulazione ab initio per giungere alle tecniche per lo studio della soft matter a livello mesoscopico. Verra' quindi mostrato come lo sviluppo della modellistica molecolare abbia permesso di trovare applicazione in settori tradizionali quali la Sintesi e caratterizzazione chimica, Ingegneria Chimica, Progettazione di farmaci, design di nuovi materiali, biotecnologie etc.
Al termine di ciascun seminario ci sara' una sessione dedicata alla discussione ed ove opportuno all'esercitazione.

Tutti gli interessati sono invitati a partecipare.
Per motivi organizzativi e' gradita una manifestazione di interesse tramite email indirizzata a fmocci@unica.it

DOVE? sala riunioni del Dipartimento di Scienze Chimiche e Geologiche. A CHE ORA? Tutte le lezioni inizieranno alle Ore 15

CHE GIORNI?	ARGOMENTO SEMINARIO
MONDAY, May 18th	**Basic Methods.** First-principles techniques and force-field-based simulation methods: How molecular interactions are described using quantum mechanics (first-principles). Introduction to several modern modeling and simulation methods
THURSDAY, May 21th	**Basic Models.** Force fields: How conceptually simple empirical force-field based models are constructed improved and optimized based on Quantum Chemistry calculations and phenomenological physical models. Strengths and weaknesses of current force fields.
TUESDAY, May 26st	**Introduction to multiscale modelling.** No single modeling method currently can be used to describe matter from electrons and nuclei to macroscopic level. Different physical models are needed at different length and time scales. We discuss here several methods and how they can be combined cover longer scales in materials modeling. Finally we discuss how to connect different scales accurately and systematically. Hierarchical coarse-graining from nuclei and electrons to mesoscale: Successive reduction of degrees of freedom is a powerful scheme to connect length and time scale. Here discuss so called inverse methods where coarse-grained models are obtained from already obtained results from an underlying detailed level.
THURSDAY, May 28th	**Approaching the macroscopic**: Lattice and field methods as well as kinetic models: When approaching the macroscopic scales in matter description particle-based models cannot be used. Here we describe several modeling methods based on materials properties not related to basic interacting units.
MONDAY, June 15th	**Applications**: Organic and drug(-like) molecules: This lecture gives an overview of molecular simulation of small molecules as liquids and in solution or in mixtures. Simulations of solvation and solubility, lipophilitiсy and permeability of organic drug-like molecules.
TUESDAY, June 16th	**Applications:** Ionic liquids: Ionic liquids are salts with organic (often large) cations and inorganic or organic anions that are often liquids at room temperatures. They have a tremendous potential in a large variety of applications due to their intrinsic properties. However, they often difficult to study both experimentally and using modeling. Here we discuss the state-of-the-art in simulation of ILs.
THURSDAY, June 18th	**Applications:** Porous materials & carbon capture and separation: Many types of porous materials, zeolites, metal organic frameworks, porous silica, carbon etc have many applications from gas purification and storage to capture and separation. We discuss here modeling of porous materials to be used in carbon (CO2) capture
WEDNESDAY, June 24th	**Applications**: Nucleic acids & proteins. Nucleic acids and proteins are the key molecules of life. Modeling them is also a big challenge. It can be done at several levels of sophistication depending on what are the properties we wish to access. Here we give a broad survey to the field.
THURSDAY, June 25th	**Applications:** Membranes and membrane proteins. The walls of cells are made of lipid membranes with polar heads and long oily tails. To model membranes and amphiphilic systems in general is less trivial as even small errors accumulate in ordered systems. However the lipid models have been improved to give good description for lipid membranes and membrane proteins embedded in them. We go through a number of examples.
MONDAY, June 29th	**Conclusion & Perspective.** Summary of state-of-the art and future outlook of computer simulations. Here we summarize the field "computational chemistry" and its potential in different areas. How do we develop simulation methods from being descriptive to become more predictive. We discuss new emerging ideas and possibilities.