

## Workshop Announcement

### **SPEAKERS:**

**Dr. Oliviero Andreussi**  
(EPFL-Switzerland)

**DrDavide Ceresoli**  
(CNR-ISTM, Italy)

**Dr. Abdallah Qteish**  
(YU-Jordan)

### **CONTACT:**

Dr. Najeh Zarir  
[najeh@sharjah.ac.ae](mailto:najeh@sharjah.ac.ae)

Dr. Iyad Al-Qasir  
[iaqasir@sharjah.ac.ae](mailto:iaqasir@sharjah.ac.ae)

### **LOCATION:**

Building M3, Room 014  
University of Sharjah  
Sharjah, UAE

### **DEADLINE:**

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### **SPONSOR:**

Office of Vice Chancellor for  
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**Second Sharjah Regional Workshop on Computational  
Science and Engineering December 11-13, 2016**

**Centre for Advanced Materials Research  
Research Institute of Sciences and Engineering  
University of Sharjah**

Computational material science is nowadays a highly developed field of research, in terms of basic theory, algorithms and applications. The first-principles computational techniques are currently being used to tackle fundamental problems in physics, chemistry, biology, geophysics, material science and nuclear Engineering. On this second workshop we will focus on Ab-Initio Molecular Dynamics (AIMD). In this approach, the atomic trajectories are computed by integrating the Newtonian equations of motion, whereas the interatomic forces are obtained on-the-fly from quantum mechanically electronic structure calculations based on density functional theory. The AIMD approach is proved to provide accurate description of thermodynamic properties and phase stability, atomic dynamics, and chemical reactions as functions of temperature. This approach takes explicitly into account bond breaking and formation. The basic theory behind this approach will be described in details. Moreover, hands-on tutorial sessions will be organized, in which the attendees can learn how to perform such simulations by using one of the most widely used packages (Quantum Espresso).

**PARTICIPATION:** Scientists from the UAE and the neighboring countries may attend the Workshop. Some knowledge of the DFT calculation and the Linux operating system will be preferred. There is no registration fee.

**HOW TO APPLY:** The online application form can be accessed on the workshop website; <http://www.sharjah.ac.ae/AIMD2016>

**SECRETARIAT:** E-mail: [Thurayah@sharjah.ac.ae](mailto:Thurayah@sharjah.ac.ae) Telephone: +971 6 5050351 Telefax: +971 6 5050352

University of Sharjah Home Page: <http://www.sharjah.ac.ae>