



International Institute for Multifunctional Materials for Energy Conversion (IIMEC)  
2012 WINTER SCHOOL IN COMPUTATIONAL MATERIALS SCIENCE ACROSS SCALES  
College Station, Texas, USA  
January 8-17, 2012

**Rationale**

Throughout history, the development of technology-enabling materials has been carried out using mostly experimental approaches. Thanks to recent advances at the theory, software and hardware level, computational materials science has emerged as an extremely valuable tool in the development of new materials.

**Goals**

The goal of this week-and-a-half Winter School is to introduce some of the most important methods within the Computational Materials Science toolkit to undergraduate and graduate students interested in this emerging field. Since materials science studies multi-scale phenomena, this Winter School will offer modules focused on different methods used to investigate physical phenomena at multiple scales.

**Organization and Topics**

Topics will be organized in a top-down approach and connections will be made between different time and length scales.

Themes will be organized as follows:

1. Mechanical response of materials: from the continuum to the mesoscale
2. Computational thermodynamics of materials
3. Evolution of microstructure at the mesoscale
4. Atomistic simulations: classical potentials
5. Calculating materials properties at the electronic structure levels

The School will consist of theoretical modules offered by experts in the field, followed by practical laboratories where the participants will have the opportunity of using the methods reviewed to simulate specific material phenomena. The newly established IIMEC Computer Cluster acquired with financial support from the National Science Foundation will be used during the hands-on sessions.

Interactions among participants is fundamental to achieve the full potential of the Winter School and social activities will be planned to provide ample opportunity to exchange experiences and ideas as well as to initiate collaborations that can be fostered within the IIMEC program.

This Winter School will be immediately followed by the IIMEC 3<sup>rd</sup> Annual Meeting, held in College Station, Texas on January 18-19, 2012.

**Application Information:**

Go to <http://www.iimec winterschool.org> to fill out the application. Final application's deadline: **November 15<sup>th</sup>, 2011.**

Applicants may be graduate students, post docs or IIMEC junior faculty.

It is recommended that international participants complete application as soon as possible.

**Financial Support:**

A limited number of full fellowships (covering registration, travel and lodging) will be made available to qualified applicants as well as a number of partial fellowships (covering registration and lodging for **non-local students**, and registration for **local students**).

**Registration Fee:** \$500.00 (Registration fee will cover teaching materials, breakfast and lunch on class days, refreshments, two banquets, two excursions, etc.).

**Organizers:**

Raymundo Arroyave, Dimitris Lagoudas, Etienne Patoor, Amine Benzerga, Tahir Cagin

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**Sponsor:**

The National Science Foundation