X Encontro da SBPMat
Gramado-RS
25 a 29 | setembro 2011

X Brazilian MRS Meeting 2011

Symposium G: Molecular Modeling Materials Science

Scope of the Symposium

The improving of hardware, software and computational techniques have been utilized in molecular modeling of complex materials including oxides, nitrides, and organic and inorganic semiconductors, paving the way to the development of new technological apparatus. The aim of this symposium will be focused on molecular modeling of materials devices and will cover topics from the fundamental theory and computational studies to modern advances in grid computing.

Abstracts will be solicited in (but not limited to) **the following areas:**

- Modeling of thin films and nanostructures
- Grid computing of materials properties
- ovel molecular modeling methods
- tructures-property relationship based on ab initio methods
- Density Functional Theory
- Monte Carlo simulation of materials
- Application of Molecular Dynamics to materials

Invited speakers

Antonio Carlos Borin (IQ - USP - São Paulo), **A. Beltran** (Universitat Jaume I - Castellón de la Plana ? Espanha), **Ney Lemke** (IBB - UNESP - Botucatu/SP), **J. Chahine** (IBILCE - UNESP - São José do Rio Preto/SP), **Fernando Luis Barroso da Silva** (FCFRP - USP - Ribeirão Preto/SP).

Symposium Organizers

Aguinaldo Robinson de Souza (Departamento de Química – UNESP)
Nelson Henrique Morgon (Instituto de Química – UNICAMP)