Symposium G

Title:

Molecular Modeling Materials Science

Scope:

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.

Session Topics:

- Modeling of thin films and nanostructures
- Grid computing technologies in materials science
- Novel molecular modeling methods
- Density Functional Theory and TDDFT
- Monte Carlo and Molecular Dynamics simulation of materials
- Relativistic Quantum Chemistry applied to materials
- Computer simulation applied to catalysis and supramolecular chemistry
- Semi empirical methods applied to materials science

Tentative List Invited Speakers:

Ataualpa Albert Carmo Braga, Universidade de São Paulo, Instituto de Química, Departamento de Química Fundamental, Brasil

Francisco Bolivar Correto Machado, Instituto de Tecnologia da Aeronáutica, Departamento de Química, Brasil

Paula Homem de Mello, Universidade Federal do ABC, Centro de Ciências Naturais e Humanas, Brasil

Léo Degreve, Universidade de São Paulo, Departamento de Química, Brasil

Luiz Guilherme Machado de Macedo, Universidade Federal do Pará, Departamento de Química, Brasil

Symposium Organizers:

Nelson Henrique Morgon, Universidade Estadual de Campinas, Instituto de Química, Brasil

Aguinaldo Robinson de Souza, Universidade Estadual Paulista "Júlio de Mesquita Filho", Departamento de Química, Brasil