

Symposium: Research Frontiers of Computer Simulations in Materials Science: Developments and Applications

Scope of the Symposium

This symposium will be dedicated to the Research Frontiers of Computer Simulations in Materials Science, which includes recent theoretical developments, algorithms, methods, theories and applications in Materials Science (nanostructures, surfaces, bulks, adsorption phenomena, complex interfaces and chemical reactivity). It is intended to be a forum where scientists from different areas in Chemistry, Physics and Materials Science merge to discuss about relevant aspects on those topics.

Our list of tentative speakers includes several world leaders in their fields, and several speakers will be selected among the best abstracts.

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

- Applications of Density Functional Theory, Hartree-Fock, and Semi-Empirical methods.
- Molecular dynamics simulation and coarse grain approaches.
- Multi-scale computational chemistry methods.
- GPU, GRID Computing and molecular modeling of materials.
- The role of global optimization algorithms and accelerated methods in Materials Science.
- Nanostructures, surfaces, bulks and complex interfaces.
- Reactions and interactions of molecular systems with surfaces.
- Renewable energy materials.
- Transparent conducting oxides.

Invited speakers:

- Roberto Dovesi, University of Torino, Italy.
- Adalberto Fazzio, University of São Paulo, Brazil.
- SuHuai Wei, National Renewable Energy Laboratory, USA.
- Klaus Capelle, Federal University of ABC, Brazil.
- Alfonso Hernández-Laguna, University of Granada, Spain.
- Edison Zacarias da Silva, UNICAMP, Brazil.
- Gerd Bruno Rocha, Federal University of Paraíba, Brazil.
- Javier Fdez. Sanz, Universidad de Sevilla, Spain

Symposium Organizers:

1. Juarez L. F. Da Silva

São Carlos Institute of Chemistry, University of São Paulo, Brazil.

2. Miguel San-Miguel,

University of Sevilla, Spain.

3. Julio Ricardo Sambrano,
São Paulo State university, Bauru, São Paulo, Brazil.