



Symposium S : Computational Design for Development of Functional Materials - Synergy Between Theoreticians and Experimentalists

Scope of the Symposium

This symposium aims to discuss research frontiers and joining studies in theoretical and experimental areas in the control and understanding of intrinsic and extrinsic properties of functional materials. The main idea is to promote discussions involving fundamental and technological aspects of materials systems that may lead to the improvement, understanding and foreseeing of the properties of technological devices. It will be desirable to gather researchers actively working in Materials Science focusing on nanomaterials with functional properties and using both theoretical methods or experimental techniques to characterize electronic and structural properties. This meeting intends to open up new opportunities to collaboration between experimentalists and theoreticians improving the ways to gain insights into the atomistic understanding of the nanomaterials. The list of invited speakers includes several world leaders in computational simulations showing how the theoretical contributions can significantly aid the experimental observations to gain a better knowledge in Materials Science. Several participants for oral contributions will be selected among the best abstracts.

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

- 1. *Computational simulation methods and experimental techniques applied to study structural and electronic properties of 1D, 2D and 3D materials*
- 2. *Applied Nanostructured materials*
- 3. *Development and application of art state computational methodologies; applied to Materials Science*
- 4. *Materials with potential application in energy generation and environment*
- 5. *Transparent conducting oxides*
- 6. *Electron-material interaction*
- 7. *Chemical reactions in materials synthesis*
- 9. *Computational design of biomaterials*
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- 10. *Theoretical insights in catalysis*

Tentative list of invited speakers (To be confirmed)

Alfonso Hernndez Laguna (*Granada University, Spain*) **Rafael Aez** (*Venezuelan Institute for Scientific Research*) **Reinaldo Pis Diez** (*La Plata National University*) **Joao Batista Lopes Martins** (*Brasilia University*) .

Symposium Organizers

Julio Ricardo Sambrano (*So Paulo State Univerity, Bauru, Brazil*) **Miguel A. San-Miguel** (*So Paulo State University of Campinas, Brazil*) **Anbal J. Rodriguez-Cuesta** (*Oak Ridge National Laboratory, USA*) **Silvia Casassa** (*Torino University, Italy*) .

<https://sbpmat.org.br/18encontro>

XVIII Brazil MRS Meeting