



Symposium AC05 : Computational Design in Materials Science, Methodologies and interplay between Theory and experiment

Scope of the Symposium

The symposium aims to promote discussions between theoreticians and experimentalists regarding the understanding of intrinsic and extrinsic properties of functional materials. The idea is to focus on the interplay between state-of-the-art computational design and experimental methodologies. Fundamental and technological aspects of materials systems that may lead to improving, understanding and foreseeing the properties of technological devices will be discussed during the event. We would like to gather researchers actively working in Materials Science, focusing on nanomaterials with functional properties and using theoretical or experimental techniques to characterize electronic and structural properties. This meeting intends to open up new opportunities for collaboration between experimentalists and theoreticians, improving insights into the atomistic understanding of 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 of Materials Science. Several participants for oral contributions will be selected among the best-submitted abstracts.

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

- *Computational simulation methods and experimental techniques applied to study structural and electronic properties of 1D, 2D and 3D materials*
- *Development and application of state-of-the-art computational methodologies in Materials Science*
- *Materials with potential application in energy storage/generation and environment*
- *Transparent conducting oxides*
- *Electron-matter interactions*
- *Chemical reactions in materials synthesis*
- *Materials Design with special optical properties*
- *Computational Design of biomaterials*
- *Theoretical insights in catalysis*
- *Related computational topics*

Tentative list of invited speakers (To be confirmed)

Aníbal J. Ramirez-Cuesta (*Oak Ridge National Laboratory*) **Juan Andrés** (*University of Jaume I*) **Norge Cruz** (*Universidad de Sevilla*) **Pablo Andrés Denis** (*Universidad de la República de Uruguay*) **Douglas Soares Galvao** (*Instituto de Física Gleb Wataghin - UNICAMP*) **Luis Henrique da Silveira Lacerda** (*Universidade Federal de Santa Catarina (UFSC)*) .

Symposium Organizers

Ricardo Paupitz Barbosa dos Santos (*Physics Department - UNESP*) **Julio Ricardo Sambrano** (*Mathematics Department - UNESP*) **Miguel Angel San Miguel Barrera** (*Chemistry Institute - UNICAMP*) **Andre Rodrigues Muniz** (*Federal University of Rio Grande do Sul - UFRGS*) .

XXII B-MRS Meeting