School of Materials Science and Engineering

Seminar Topic: Computational Materials Science at Sorbonne University

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Abstract

Computational approaches are nowadays a full, self-standing branch of materials science, both for their quantum-based (“ab initio”) accuracy, and for their multi-scale extent. In this talk I will present an overview of Computational Materials Science (CMS) research at Sorbonne University. In the first part, I will starting with fundamental questions, such as the Topological-based definition of Global Coordinates capable to describe and predict, at the ab initio level, transformations thermodynamics, kinetics and mechanisms in materials. In the second part, I will present several axes of research of our group at SU, including technologically relevant glasses, CO2 behavior, reactivity and storage, supercapacitors, battery-electrodes, topological materials, nanomaterials.

Biography

Dr A. Marco Saitta obtained a Laurea in Fisica from the University of Messina (Italy) in 1994, then a PhD in Condensed Matter Theory from the International School for Advanced Studies (SISSA/ISAS) in Trieste in 1997. He then moved to Philadelphia, USA, for a postdoctoral position at the Department of Chemistry of the University of Pennsylvania (Ivy League). In 2000, he was appointed Maître de Conférences at Université Pierre et Marie Curie (UPMC), at the Physique des Milieux Condensés laboratory, now Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC) in Sorbonne University. He acceded to Professorship in the same lab in 2011, to 1st class Professorship in 2014, and to “Exceptional class” in 2017.

A specialist of electronic structure theory and ab initio calculations, his research activity has spanned from bulk semiconductors to graphene and nanotubes, to water and ices. His main interests being the exotic properties of molecular crystals, liquids and amorphous at extreme conditions of pressure and temperature, for which he has received in 2006 the Young Scientist Award from the European High Pressure Research Group.

In recent years his research has opened up into more interdisciplinary fields, such as Earth sciences and Geochemistry. He has authored about 100 articles, including 1 Nature, 2 Nature Materials, 1 Nature Communications, 7 PNAS, and 19 Phys. Rev. Lett. He has about 4000 citations, an h-index of 33.

Thursday, 28 March 2019 || Time: 11:00 am – 12:00 pm || Venue: MSE E-Studio (N4.1-B2-02)

Hosted by: Assistant Professor Martial Duchamp

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