Laboratoire des Solides Irradiés, UMR 7642

Séminaire Invité

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Mardi 7 Juin 2016 – 16h00
Salle de réunion LSI (bâtiment 83)

Efficient Linear-Scaling Approaches to Electron Transport in Condensed Matter Systems: Charge, Spin and Hall Transport

The number of intriguing electronic materials is exploding with completely new emerging classes that have been unknown few years ago. Among them, Topological Insulators, Weyl Semimetals, 2D Materials, or novel Organic Semiconductors are discussed regarding specific transport properties. Theoretical approaches can describe the electronic properties in such emerging materials. However, the understanding of charge transport properties is a much more challenging endeavor because it can be influenced by disorder or other perturbations invisible to optical spectroscopy. At an early stage of novel materials, this clearly demands strong support by transport simulations studies. However, from the theoretical side there is currently only little support because efficient approaches are lacking for transport. Current tools either suffer from a lack of accuracy or scale badly with the system size.

In this presentation, I will introduce a method that aims at closing this gap of current research. I will demonstrate for few cases how large-scale charge transport and spin transport simulations based on the Kubo method in combination with accurate electronic-structure simulations can lead to an in-depth understanding of transport signatures which remain otherwise unexplained.

Short-BIO: Frank Ortmann received his doctorate with “summa cum laude” from the Friedrich Schiller University Jena (Germany) in 2009 with a dissertation on the theory of charge transport in organic semiconductors. In the same year he joined CEA Grenoble (France) as postdoctoral fellow and was awarded a Marie-Curie Fellowship in 2010. In 2011 he moved to the Catalan Institute of Nanoscience and Nanotechnology, Barcelona (Spain). In 2013 he joined the TU Dresden (Germany), where he is now leading an Emmy Noether young investigator group since 2014.