TECHNISCHE UNIVERSITÄT
CHEMNITZ

Institut für Physik
Physikalisches Kolloquium

Mittwoch, 06.01.2016, um **16:00 Uhr**

Ort: Reichenhainer Str. 90;
Zentrales Hörsaal- und Seminargebäude, Raum 2/N013

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From Electronic Structure to Charge- and Spin-Transport: A Story in Three Parts

The number of materials in research 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. For such emerging materials, many computer codes readily implement theoretical approaches such as density functional theory to describe electronic properties which can be directly compared to measurements from angle-resolved photoelectron spectroscopy. Materials discovery projects make use of such simulation tools by screening huge numbers of material candidates for their electronic properties to select a subset for further experimental studies.

On the other hand, the understanding of charge transport properties of emerging materials in experiment is a much more challenging endeavor because it can be influenced by disorder or other perturbations invisible to spectroscopic probes. At an early stage of new materials, this clearly demands great support from theoretical studies as material quality needs to be improved. However, from the theoretical side there is only little support because approaches analogous to DFT 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.

Alle Zuhörer sind ab 15:45 zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt:
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