



e-conversion



# Seminarankündigung

**Dienstag, 8. Juni 2021**

**17:00 Uhr**

**ONLINE via ZOOM**

## **“From charge and spin transport to excitons in solar cells: Insights from efficient approaches for linear response functions”**

The number of interesting electronic materials is constantly growing and completely new classes are emerging that were unknown a few years ago, including topological insulators, Weyl semimetals, 2D materials and novel organic semiconductors. For such emerging materials, electronic-structure theories can describe electronic properties that can be directly compared with measurements from angle-resolved photoelectron spectroscopy or probed locally by scanning tunneling spectroscopy. Understanding electron transfer and charge transport properties, however, is more complicated. This is because it requires describing disorder, vibrations and their effect on propagating electrons. In addition, typical transport geometries require the simulation of large systems, since the transport properties depend on the size of the system or just because of large unit cells as for instance in polycrystalline or Moiré systems. Unfortunately, current tools suffer from a lack of accuracy or scale badly with the system size.

In this presentation, I will introduce linear-scaling approaches that can close this gap. I will demonstrate, for selected cases, how large-scale charge-transport and spin-transport simulations based on the Kubo framework in combination with electronic-structure simulations can lead to an in-depth understanding of various transport signatures that would otherwise remain unexplained.

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