Sonderforschungsbereich 1277

Emergent Relativistic Effects in Condensed Matter -
From Fundamental Aspects to Electronic Functionality

SFB – Colloquium

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Date: Tuesday, 18.06.2024, 14:15, H34

Topic: Wonders and Wanders in Density Functional Theory Applied to van der Waals Materials

Abstract:

In recent years, there has been a widespread and intense interest in the determination of electronic structure and optical properties of two-dimensional van der Waals (vdW) materials. This is due to their potential impact in a vast number of scientific fields and technologies, ranging from nanoelectronics to photovoltaic and photocatalytic applications. Accurately predicting these properties from first principles is an outstanding challenge.

In this talk, I will discuss how this challenge can be overcome using density functional theory (DFT). I will present how to accurately determine the electronic structure, as well as the optical absorption spectra of low-dimensional vdW materials with DFT and (Wannier-localized optimally-tuned) screened range-separated hybrid functionals [1, 2]. The parameters defining these functionals are material- and structure-dependent. I will show a non-empirical process of determining the functional parameters and I will apply it to prototypical vdW materials. The obtained electronic and optical properties display a level of accuracy comparable to that of ab initio many-body perturbation theory.

[1] M. Camarasa-Gómez, A. Ramasubramaniam, J. B. Neaton, L. Kronik, Phys. Rev. Materials **7**, 104001 (2023).
[2] M. Camarasa-Gómez, Stephen E. Gant, G. Ohad, J. B. Neaton, A. Ramasubramaniam, L. Kronik, arXiv:2405.00643 (2024).

Host: Prof. Dr. Ferdinand Evers