CENIDE & WIN Seminar Series on 2D-MATURE

DFG IRTG 2803 & NSERC CREATE

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"A novel density functional theory approach for 2D materials"

May 22nd, 2025
10:00 a.m. ET / 16:00 p.m. CET

Michael Lorke studied physics at the University of Bremen, where he got his PhD in 2009. After a PostDoc stay at DTU in Denmark, he returned to the University of Bremen where he worked on a crossroad between material physics and theoretical physics. Since 2024 he holds a DFG position at the University of Duisburg-Essen.

Density functional theory is the workhorse of theoretical materials investigations. Due to the shortcoming of (semi-)local exchange correlation potentials, hybrid functionals have been established for practical calculations to describe surfaces, molecular adsorption, and defects. These operate by mixing between semi-local and Hartree-Fock exchange semi-emprically. However, their parameters have to be optimized for every material separately. To treat materials with a more physics driven approach and without the need of parameter optimization is possible with many-body approaches like GW, but at an immense increase in computational costs and without the access to total energies and hence geometry optimization.

We have introduced an exchange correlation potential for semiconductor materials, that is based on physical properties of the underlying microscopic screening. We demonstrate that it reproduces the low temperature band gap of several materials and show that it can be used as a kernel in linear response TDDFT to reproduce excitonic effects in optical spectra. We will discuss how to generalize such a functional to anisotropic systems like 2D materials. The presence of interfaces modifies the screening behavior in layered systems in a way, which cannot be described by HSE or any other screened exact exchange functional, which are based on assumptions of isotropy. Since even state-of-the-art many-body calculations must be based on a-priori defect geometries obtained by LDA, GGA, or a hybrid functional, at present there is no method available to achieve the same accuracy in mono- and few-layer systems as for the bulk.

We will also discuss results from an experiment/theory collaboration with the TU Munich on single-photon sources in MoS2 and show how to combine DFT calculation with many-body theory to reproduce experiments over a wide temperature range.