Carl von Ossietzky
Universität
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Theoriekolloquium

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https://meeting.uol.de/b/and-etc-jmj-1y9

Am **6. Mai 2021 um 14.15 Uhr** hält

Herr Dr. Michael Lorke (Bremen)

einen Vortrag mit dem Titel

Optoelectronic properties of nanostructured devices

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 functionals operate by mixing between semi-local and Hartree-Fock exchange semi-empirically. 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 access to total energies and hence geometry optimization.

We propose a novel 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. Moreover, on the example of defects in semiconductors, it respects the required linearity condition of the total energy with the fractional occupation number, as expressed by the generalized Koopman's theorem. We show, that it also serves as a useful kernel for TDDFT to calculate excitonic effects in semiconductors.

We will also discuss quantum light sources in transition metal dichalcogenides. These can, e.g., be tailored through deterministic defect engineering. A major difficulty is that defects need to be positioned site-selectively within the solid. We show controllably generated defects in single-layer MoS2 using a sub-nm focused helium ion beam. Based on ab-initio calculations we interpret these emission lines as stemming from the recombination of highly localized electron-hole complexes at defect states, generated by the helium ion bombardment. Using a many-body approach for dephasing due to electron-phonon interaction, we quantify the spatial extension of the emission centers and compare them to the results of the ab-initio calculation. As an alternative approach, we discuss a different platform, which consists of TMD nano-bubbles that develop if air is enclosed during the stacking of layers. Due to the high bending rigidity, strain induces large variation of the band-gap that can lead to carrier confinement. Another, much less discussed, mechanism is the change of the dielectric environment that also induces strong band-gap variations.

Interessierte sind herzlich eingeladen.

gez. Prof. Dr. Caterina Cocchi