# Understading semiconductor defects

## High-level calculations on defects and surfaces of semiconductors

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### In Short

- Find optimized functionals to calculate the electronic structures of defects in Ga-base semiconductors.
- Investigate defects in relevant Ga based 2D- and 3D-seminconductors using the optimized functional.
- Develop an efficient method to deal with the artefacts usually appearing in calculations with charged defects.

The functionality of semiconductors is closely connected to their defects, which control the electronic and optical behavior of the bulk material and the chemical behavior of the surface. While the standard local (LDA) and semi-local (GGA) approximations of density functional theory (DFT) have played an important role in understanding the properties of defects in traditional semiconductors, they often fail completely in wide band gap materials. In recent years, screened hybrid functionals (mixing non-local and semi-local exchange), like HSE06, have emerged as a possible replacement. The present project deals with the application, refinement and possible extension of HSE-type functionals for defects and surfaces of wide band gap semiconductors. We have found earlier that semi-empirical, material-specific tuning of the two parameters of HSE (i.e., the fraction of non-local exchange, $\alpha$, and the inverse screening length, $\mu$) can lead to a good approximation of the exact functional, and allows the calculation of defect levels in the gap with an accuracy of 0.1 eV. While the optimized parameters work well for all defects within the given host, the transferability of the parameters to other materials is very limited. In the framework of our running DFG-project Defect calculations in Ga-based semiconductors using optimal hybrid functionals (FR2833/63-1), we have found, e.g., that CuGaS2 and CuGaSe2 can be well described with the same pair of parameters, but replacing Ga with the chemically similar In requires new ones. Therefore, in the past project year we have mapped the optimal parameter field for a series of Ga-based semiconductors, spanning a gap range between 1.4 and 4.7 eV. We will use the obtained knowledge to design an improved semi-empirical hybrid functional (with a better description of screening), having parameters transferable across the chosen set. We have modified the VASP electronic structure package, making it possible to utilize more general screening functions, and in this project year we would like to test various possibilities.

Our goal in the project is also to use the optimized HSE($\alpha$,$\mu$) functionals to solve application-relevant defect problems in wide band gap semiconductors. In the first project year we have published new results on defects of GaN and $\beta$-Ga2O3, two materials with high importance for power electronics and opto-electronics. As mentioned above, the crucial point in the success of the screened hybrid functionals is the description of screening. From this point of view, surfaces and, especially, two-dimensional materials represent a challenge because of the highly anisotropic screening behavior. Therefore in the second year of our present HLRN project, we would like to extend our investigations to such systems. On the one hand, we intend to use a single-atom sheet of the wide band gap hexagonal boron nitride (h-BN), as a test case for 2D materials and, on the other hand, we will study the layered semiconductor GaSe, which is relevant for non-linear optics application. Using an HSE($\alpha$,$\mu$) functional, optimized for bulk GaSe, we will carry out practical defect calculations, and will check, how the performance of the optimized hybrid, and the defect properties change, when going from the layered bulk material to a single layer.

Calculation of charged defects in layer or slab require corrections to eliminate the interaction of the artificially repeated charges. In the first year of the project we have also continued our work toward a self-consistent and general charge correction scheme. We have completed a stand-alone, parallelized code for calculating the correction of the

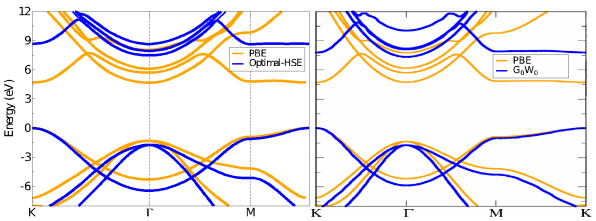


***Figure 1:** The band gap of h-BN between special points of the Brillouin zone. The yellow lines are the result of a GGA calculation (using the PBE functional). The blue lines come from the optimized hybrid on the left and from a first-principles G0W0 calculation on the right.*

total energy even for complicated charge distributions. The results obtained by this code can now be used to test self-consistent versions built into standard electronic structure packages, like Quantum Espresso or VASP. So far we have experimented with two different strategies and expect the better one to be functional by the second half of the project year. We have completed a stand-alone, parallelized code, SLABCC, for calculating the correction of the total energy even for complicated charge distributions. In the framework of our other running DFG project: "Theoretical and experimental study of charge transfer processes in photocatalysis on anatase-TiO2" (DE1158/8-1), we have tested the program by investigating the photocatalytic oxidation of CO. The results obtained by SLABCC can now be used to test self-consistent versions built into the standard electronic structure packages, like Quantum Espresso or VASP. So far we have experimented with two different strategies and expect the better one to be functional by the second half of the project year. Then we will study the photo-assisted adsorption of NO2 on anatase-TiO2, a basic step in processes relevant for environment protection.

## WWW

http://www.bccms.uni-bremen.de

## More Information

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