

Dynamics and Interactions of Semiconductor Nanowires for Optoelectronics

DFT and Many-Body investigations of functionalized semiconductor nanowire structures

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In Short

- Functionalization of GaN.
- RE and TM doping of semiconductor nanowires.
- Modification of electronic and optical properties.

The main objectives of this project are the functionalization of Gallium nitride and doping of Zinc oxide nanowires in order to investigate their electronic and optical properties by using first principle density-functional theory (DFT) and many-body methods (GW and Bethe-Salpether equations). One possible approach for the necessary surface modification of Gallium nitride is the attachment of functional groups to the nanowire surface. In addition, rare-earth (RE) and transition metal (TM) elements will be used to modify the electronic and optical properties of the nanowires to investigate their suitability for optoelectronic devices such as lasers, LEDs or single-photon sources.

The scientific and technological interest in functionalizing the surface of semiconductor nanostructures with organic molecules has grown over the past years, since this could lead to hybrid materials with desired properties to be used in solar cells or LEDs. Since the chemistry of the interfaces between the nanostructure and the molecules (groups) is tough to determine, it is still not clear, which groups are best suited for surface modifications and how exactly they affect properties like charge transfer and conformation energies. So one key aspect for the functionalization is to understand the semiconductor-organic interface.

In preceding work, we have investigated doping of ZnO and will continue to do so. In particular, Europium is only optically active in its 3+ oxidation state, whereas its formal charge in ZnO amounts to 2+. We have investigated Eu in the presence and absence of intrinsic defects. As an example for a simple intrinsic defect, an Europium-Oxygen vacancy complex is shown in Fig. 1.

The corresponding electronic structure is presented in Fig. 2.

In this subproject, the material system Gallium nitride (GaN) will be focused since it is of high interest to the research unit FOR1616. Out of the

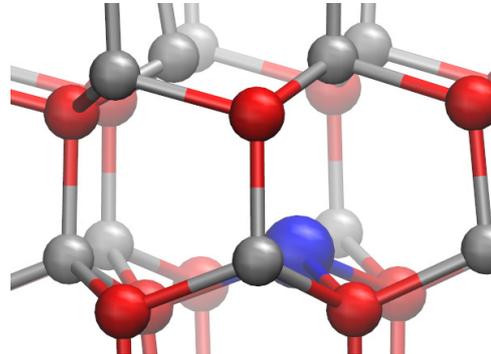


Figure 1: Eu-O vacancy complex. Red, grey and blue balls represent O, Zn and Eu ions.

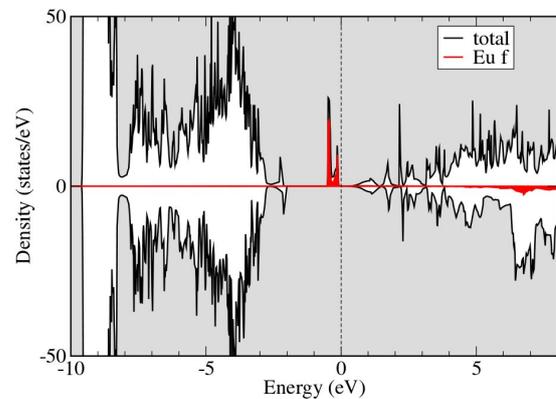


Figure 2: Electronic structure for Eu incorporated on a Zn position in ZnO, next to an oxygen vacancy, calculated using the GW0 approximation. The dashed line denotes the Fermi energy.

investigated semiconducting materials, GaN is the toughest for chemical modifications, because it has to be etched prior to the organic modifications. Furthermore the atomic structure has to be determined precisely before any functionalization can take place. Similar to the procedure in ZnO, this involves the determination of the most stable adsorption structure and to verify the energetic stability. DFT and DFTB calculations will be used to investigate these purposes. In addition during the functionalization procedure the electronic structure of the most stable configuration will be determined using hybrid functional and many-body methods.

The optical properties for the energetically stable configurations of those systems can be calculated using many-body methods as soon as the equilibrium structures have been determined. The GW approximation as well as the Bethe-Salpeter equation will allow the calculation of quasi-particle spectra,

optical spectra and exciton binding energies. Those can become fundamentally important to describe and understand the exciton creation and its spatial charge separation in holes and electrons.

WWW

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

More Information

- [1] Many-Body electronic structure calculations of Eu doped ZnO. M. Lorke, T. Frauenheim and A. L. da Rosa, *submitted to Phys. Rev. B*.

Project Partners

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