O 24: Poster Session - Electronic-Structure Theory: General

Time: Monday 18:15–20:00 Location: P1A

O 24.1 Mon 18:15 P1A

Surface influence on the electronic properties of GaAs(001) — •Isaac A. Ruiz-Alvarado[1], Alfonso Lastras-Martínez[1], and Milton Muñoz-Navia[2] — [1]IICO, UASLP, San Luis Potosí, México — [2]CONACYT-IFUASLP, San Luis Potosí México

Tailoring materials properties nowadays requires alloying individual properties. Due to its open scientific questions and technological implications, combining Ga and As (GaAs) is a long standing binary system of interest. Recently, the Reflectance Difference Spectroscopy (RDS), has re-emerge as a powerful technique to characterize and monitor the specific in situ growth in surfaces. However, for the system of interest (GaAs), in the literature several possible surface reconstructions are proposed. The physics behind the optical anisotropies related to the surfaces is an open question and not yet resolved with (RDS). Understanding the physics that gives rise to the reconstruction of GaAs (2x4) surface, and its implications in the (RDS), is interesting from a scientific and technological point of view. In this work, we discussed the structural energy landscape of several possible reconstructions in GaAs (2x4) surface. In the framework of a density functional theory using projector-augmented-wave method, with an exchange correlation potential in the form of the generalized gradient approximation (GGA), the electronic structure of the different surface reconstructions (namely α, $\alpha 2$, β, $\beta 2$ and $\beta 3$) are obtained. Our results show that the energy landscape of the surface reconstructions of the GaAs system can be discuss in terms of the layer by layer mobility influence and the dependence in the concentration (As or Ga rich structure).

O 24.2 Mon 18:15 P1A

Complex contour integration in non-equilibrium Green's function formalism — •Jonas Fey[1], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

In a previous work we introduced a new method for calculating the electronic density as a partial step in a self-consistent algorithm using Green's functions by calculating a non-equilibrium occupation function for complex-valued energies. In order to calculate the density in the non-equilibrium steady state Keldysh formalism, one needs a high amount of computational effort, since the integration is along the real energy axis. Going to the complex plane allows for less computational effort, but the non-equilibrium occupation function is needed. The calculation of this function worked well for a single step and indicated the possibility to make electronic structure calculations more efficient. The validity for a complete self-consistent calculation remains open. Therefore, we tested the method for different model systems simulating for example a potential barrier or a quantum dot. We investigated the correctness of our results as well as the convergence depending on the number of energy points. Furthermore, we studied analytic properties of the functions used which are crucial for the functionality of our method.

O 24.3 Mon 18:15 P1A

AiiDA workflows in KKR-DFT for high-throughput computations — •Irina Heinz[1], Philipp Risius[1,2], Alexander Fabian[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Zentrum für Materialforschung (LaMa), Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Magnetic tunnel junctions (MTJs) have seen several industrial applications over the years. Most ab initio descriptions focus on a 1×1 slab of material owing to constraints in computational time. However, supercells are necessary to describe interesting physics resulting from k-scattering. Skyrmionic structures, for example, may modulate tunnel magnetoresistance due to scattering between parts of the Brillouin zone [2]. At finite temperatures, atomic displacement and magnonic excitations are expected to contribute to the intricate effects in MTJs. However, such effects are highly material dependent. We develop workflows using a plugin for the AiiDA framework to automatically calculate transport through supercells of various materials with different types of disorder. This work paves the way for future high-throughput searches for promising material combinations.

[1] Pizzi, Giovanni, et al. "AiiDA: automated interactive infrastructure and database for computational science." *Comp. Mater. Sci.* **111** (2016): 218-230.

[2] Schäfer-Richarz, Jonas Friedrich, et al. "Magnetic tunnel junctions: An efficient way for electrical skyrmion detection investigated by ab initio theory." *Phys. Rev. B*, accepted.