

nanoSeminar Series 2022

Institute for Materials Science

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Institute for Materials Science, TU Dresden

Functionalizing phosphorene towards bipolar magnetic semiconductors

Thursday, August 11th 2022

13:00 – 14:00

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL)

Conference link: <https://tinyurl.com/nanoSeminar-GA>

Functionalization of two dimensional (2D) materials is an approach to enhance their versatility, either for improving their stability in certain conditions or tuning their properties in a desired direction. In this work we report the electronic and magnetic changes of phosphorene, a 2D material that has shown outstanding properties such a high carrier mobility and layer-dependent band gap, after functionalization with hydroxyl and cysteine molecules. We systematically studied the effects of single molecule functionalization, functionalization direction, functionalization coverage and molecular chirality can play in the electronic structure and magnetic properties of phosphorene. The main factor that plays a role in the induced electronic and magnetic changes in our phosphorene-based system is the formation of a dangling bond in a phosphorus atom after molecular functionalization. We showed that the electronic band gap, exchange splitting and other electronic structure properties can be tuned by the functionalization direction and coverage. Moreover, the functionalization with the chiral molecules showed a correlation between the magnetic ground state and chiral-composition of the functionalized molecules. The resulting systems are proposed to be employed as bipolar magnetic semiconductor (BMS) due to their characteristic spin resolved band structure. We compared the energy parameters that define a BMS and found adequate trends that improves them with that desired application for future spintronic devices.

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Alvaro studied Nanotechnology engineering at the Autonomous University of Queretaro (UAQ), in Mexico. In 2016 he got his degree with the thesis project "Synthesis and characterization of Ag-TiO₂ nanoparticles for the disinfection of wastewater" under the supervisor of Dr. Karen Esquivel. In October of the same year he started his master course "Nanobiophysics" at the Biotec of TU Dresden. For his master thesis he joined the group of Prof. Gianarelio Cuniberti under the supervision of Dr. Rafael Gutierrez, where he worked on computational studies of heat transport in nanoscale engines. Since October 2018, Alvaro is a PhD student in our group in collaboration with the International Max Planck Research School.