Science Program presents

A Journey Through the Nano Wonderland by Quantum Simulations

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This will be a voyage through the one-, two- and three-dimensional wonderlands using density-functional theory and similar quantum methods. Molybdenum sulfide nanowires are possible alternatives of carbon nanotubes with their comparative mechanical strength and similar electronic properties [1]. How could these nanowires function as nanometer-sized potentiometers or conductors? [2] Contacts of a transistor channel with electrodes have an important role in overall transistor characteristics. However, gold as a common electrode material in nanosystems establishes only weak contacts with both graphene and pop transition metal chalcogenides. Does a better alternative to gold exist? [3] Electronic transport properties of graphene are very unstable even when small amount of defects introduced. What happens with electronic properties of graphene upon its contacting with topological insulator, the material which exhibits extremely robust electronic transport properties? [4] The so called d-zero magnetism, i.e. emergence of magnetic moment in systems without magnetic elements is an open question. Existence of local charge and electric dipole is impossible in metals due to their high electron density and strong screening. Our quantum calculations predict that magnesium hexaboride has a magnetic moment which coexists with antiferroelectric order [5]. How is it possible in the metallic system without magnetic elements? We will try to find answers to these and other questions in the presentation.

"Unique structural and transport properties of molybdenum chalcocohalide nanowires"
"Electromechanical switch based on MoS2 nanowires"
"Designing electrical contacts to MoS2 monolayers: a computational study"
"Proximity-induced topological state in graphene"
"Magnetism and antiferroelectricity in MgB2"