Electronic and magnetic properties of two-dimensional crystals of transition metal iodides encapsulated by graphene

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In the last decade, one can observe rapid progress in the development of physics and nanotechnology of two-dimensional (2D) van der Waals materials. This opens a new gateway for applied science, especially for the development of 2D nanoelectronics. Our project is focused on this kind of materials, and we will investigate the electronic, magnetic, and transport properties of transition metal (TM) iodides encapsulated by graphene layers: $Gr/XI_n/Gr$ for (n = 1, 2, 3 and X = V, Cr, Mn, Fe, Co, Ni, Cu). Sandwiching the iodide layers between graphene is expected to stabilize the structure of the iodides, and also to lead to novel and unique properties of these two-dimensional materials. Graphene is a single atomic layer of carbon atoms. It is also well-known in condensed matter physics for its excellent transport properties, very high mechanical strength, and many other properties. It also plays a significant role in our project. The importance of graphene follows not only from the stabilization of iodides, but also from its interaction with the iodides, which may lead to novel and innovative electronic, magnetic, and transport properties. Additionally, the modification of the electronic and magnetic properties of these hybrid materials can also be made externally. In this project, we will use strain, external electric field, or twisting the graphene layers to control the behavior of these hybrid materials and reach at the end the demanding and required properties, useful for specific applications in nanoelectronic devices.

It has been estimated that in 2030, the global electricity demand for data centres will reach around 2.967 TWh, which is clearly a huge amount, and this requires the development of energy-efficient technologies. One of the significances of our project in that respect consists in designing and characterizing new materials, that can serve as a platform for new devices consuming less power and with ultra-fast speed at the same time. This is a significant contribution towards creating an environmentally friendly and green world, and this is in parallel with the global community efforts to reduce energy consumption and decrease environmental impacts. To achieve these project objectives, we will use advanced computational methods to predict and design the new structures, and then to investigate the electronic, magnetic, and transport properties as key properties required in practical applications.

The calculations will be based on the first-principles approach, whose purpose is to predict and design the structure using the Schrodinger equation. There exist some techniques to solve these many-body (high number of atoms inside the material) problems, and our calculations will be based on the Density Functional Theory (DFT) technique, which is well-known for its high accuracy and efficiency.

Summarizing, this project aims to explore the novel and unique properties, as well as potential applications, of TM iodide materials encapsulated between graphene monolayers. The output of this research is expected to have a significant impact on material science and on designing new devices based on the studied materials in order to reduce power consumption, which supports a green world and innovative future.