

Electronic and Magnetic Properties of Graphene-Encapsulated Transition-Metal Iodides

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By stacking distinct two-dimensional (2D) crystals, van der Waals heterostructures can host proximity effects and emergent states that are absent in the individual constituents [1]. An important strategy in such structures is graphene encapsulation, which can stabilize fragile 2D layers and simultaneously modify their electronic and magnetic properties through the proximity coupling [2-5].

We present results of our study of electronic and magnetic properties of a new class of van der Waals heterostructures based on transition-metal iodides encapsulated by graphene (Gr), i.e., Gr/XI_n/Gr (X = V, Cr, Mn, Fe, Co, Ni, or Cu); *n* denotes the number of iodine atoms in the unit cell [6]. In these systems, graphene layers act both as an encapsulating layers and as an active component that modifies the electronic and magnetic properties of the encapsulated material. Using first-principles density functional theory calculations, we analyze structural stability, magnetic ground states, and key electronic characteristics of Gr/XI_n/Gr heterostructures, including spin-dependent effects and band alignment. We further demonstrate that strain and electrostatic gating provide efficient control of the electronic and magnetic properties of these systems.

References:

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