Electric and Magnetic Properties of FeI_2/Graphene Heterostructures from First Principles

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Abstract. Two-dimensional magnetic materials have recently attracted significant attention due to their potential applications in spintronics. Transition metal dichalcogenides show diverse magnetism due to reduced dimensions, strong electronic correlations, and spin-orbit coupling. When combined with graphene, such materials form systems in which electronic, magnetic, and vibrational properties can be significantly altered by proximity effects and van der Waals pressure. In this work, we study monolayer FeI_2 encapsulated in graphene, focusing on its electronic structure, magnetism, and lattice dynamics. Electronic properties are investigated using first-principles density functional theory. Based on Wannier interpolation, we constructed an effective description that allows for a detailed analysis of magnetic behavior. Phonon spectra are studied using a supercell approach, revealing modifications induced by graphene encapsulation and the resulting van der Waals pressure. The magnetic hysteretic response of the system is further analyzed considering a decomposition into a diamagnetic and paramagnetic contributions, attributed to graphene and its defects, and ferromagnetic component that likely originates from a multi-component ferromagnetic phase of FeI_2.

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