Ferroelectric Control of Electronic Properties in a 2D CrI_2/α-In_2Se_3 Heterostructure

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The electrical control of magnetic and electronic properties remains a key challenge for next-generation low-power spintronic and optoelectronic devices. Two-dimensional (2D) materials provide an ideal platform, as their reduced dimensionality enhances interfacial effects and enables the engineering of novel functionalities through van der Waals heterostructures. In these systems, the band alignment plays a central role, governing charge transfer, carrier separation and recombination dynamics, and ultimately determines the efficiency of optoelectronic and photovoltaic processes [1]. Achieving reversible control of band alignment via ferroelectric polarization would enable non-volatile electrical tunability of interfacial properties. In particular, combining 2D magnetic and ferroelectric layers offers a promising strategy to tailor magnetism and band alignment through interfacial strain, charge redistribution, and built-in electric fields [2].

Among 2D ferroelectrics, In_2Se_3 stands out due to its robust room-temperature ferroelectricity, sizable and bistable non-volatile intrinsic polarization reversible at low voltages [3]. The large built-in electric field at In_2Se_3-based interfaces provides an efficient route to engineer charge transfer and electronic reconstruction when combined with 2D magnetic materials. Understanding how such polarization fields influence magnetic stability and band alignment at the interface is therefore essential for the rational design of multifunctional heterostructures.

Here, using first-principles density functional theory calculations, we investigate the structural, electronic, and magnetic properties of a CrI_2 monolayer interacting with ferroelectric In_2Se_3. We analyse how the strain induced at the interface stabilizes a Néel-type antiferromagnetic configuration, which is absent in the isolated CrI_2 monolayer. We further examine the influence of the In_2Se_3 polarization on magnetism and the interfacial charge transfer. Our results show that when the ferroelectric polarization of the In_2Se_3 is reversed, the band alignment of CrI_2/In_2Se_3 switches from a straddling (type I) to a staggered (type II) configuration, and the band gap changes from an indirect gap (0.89 eV) to a direct gap (0.65 eV). These findings reveal a polarization-switchable band alignment mechanism, positioning the CrI_2/In_2Se_3 heterostructure as a promising candidate for multifunctional spintronic and optoelectronic applications.

Referencias

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