Twist-Angle-Controlled Proximity Effects in Graphene on Cr-Based Magnetic Trihalides

Mirali Jafari[1] and Anna Dyrdał[1]

[1] *Faculty of Physics, Adam Mickiewicz University in Poznań, ul. Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*

Using the density functional theory, we analyse proximity-induced electronic and magnetic properties of graphene deposited on chromium-based trihalides, CrX_3 (X = Cl, Br, I). Both untwisted and twisted graphene/CrX_3 heterostructures are considered. We consider how the proximity-induced exchange interaction and spin–orbit coupling originating from the magnetic trihalides modify the electronic states of graphene, leading to spin splitting, gap opening, and valley-contrasting effects. We show that the magnitude and symmetry of these proximity effects depend on the stacking geometry, twist angle, and lattice deformations such as strain. In addition, we investigate the role of an external gate voltage in controlling valley-contrasting effects [1,2].

We also present results for graphene deposited on Janus chromium trihalide monolayers, X_3–Cr_2–Y_3 (X, Y = Cl, Br, I), in which broken structural inversion symmetry further enhances spin–orbit coupling and leads to a strong sensitivity of magnetic properties on mechanical strain [3]. Moreover, the presence of an intrinsic electric dipole moment provides an additional control parameter for graphene-based van der Waals heterostructures [4].

For selected stacking configurations, we derive an effective low-energy Hamiltonian describing the electronic properties of graphene near the K and K' points and demonstrate that the relative twist between graphene and the CrX_3 monolayer provides an efficient means to control spin polarization, topological band features, and valley-contrasting phenomena. Finally, we discuss possible topological phases and strain- or gate-driven topological phase transitions in these structures.

References:

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