Electronic and magnetic properties of van der Waals materials: first-principles studies

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Van der Waals materials are highly promising for the development of future nanoelectronics due to easy tuning and control of their magnetic and electronic properties by external strain, gate voltage, twisting of layers in heterostructures, intercalation, and others - down to the monolayer scale [1, 2]. All this allows the design of new efficient spin valve systems, ultra-low power logic elements, RF oscillators, and quantum-ready platforms [3, 4]. In this talk, I will present a route from fundamental modelling to device concepts, based on our recent studies. I will begin with two-dimensional VSe2, where we have shown that bilayers of these crystals have the potential to be used as spin-valve systems [5]. Then, I will discuss VX2 (X = S, Se, Te) monolayers and bilayers as candidates for possible applications. Using first-principles calculations together with minimal spin models, we evaluated their electronic structure as well as static and dynamic properties [6]. We focused on the T-phase VS2 bilayer and investigated how the tensile and compressive strain can modify the magnetic anisotropy energy, interlayer exchange couplings, and other relevant properties [7]. Finally, I will focus on our recent work on the proximity effect in twisted graphene on CrI3 monolayer within first-principles study and a low-energy effective model. In such a system, twist angle, pressure, and strain can tune the proximity exchange coupling, valley polarisation, and topological transport in graphene, which enables the design of novel, efficient spin- and valley-based nanoelectronics devices.

References

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