Chapter 7

Concluding remarks and Future prospect

7.1 Thesis Conclusion

The evolution of low-dimensional materials has frequently revolutionized new intriguing physical standards and suggests a unique approach to scientifically design a novel device. However, scaling down of spin-electronic devices entails in-depth knowledge and precise control on engineering interfacial structures, which unveils the exciting opportunity. To reveal exotic quantum phases, atomically thin two-dimensional van der Waals material, embraces control and tuning of various physical states by coupling with peripheral perturbation such as pressure, photon, gating, Moire pattern and proximity effect. In this thesis, we discuss the physical property of a pristine material which can be converted via proximity effects to attain intrinsic spin-dependent properties from its adjacent material like magnetic, topological or spin–orbit phenomena. Realizing magnetic proximity effect in atomically thin vdW heterostructure not only balance the traditional techniques of designing quality spin interface by doping, defects or surface modification, but also can overcome their restrictions for modelling and fabricate novel spin-related devices in nanoscale phases. The proximitized van der Waals heterostructure systems unveil properties, which cannot be realized in any integral component of considered heterostructure system. These proximitized van der Waals material provide an ideal platform for exploring new physical phenomena, which delivers a broader framework for employing novel materials and investigate nanoscale phases in spintronics and valleytronics. The featured conclusions of the current doctoral thesis are highlighted below in following points.

(a) Spin-dependent electronic properties and ballistic transport in graphene and ferromagnetic $CrBr_3$ vdW heterostructure system is realized and establishes magnetic proximity effect. At optimum interlayer distance of 3.77 Å, the magnetic proximity effect arising from the spin-dependent interlayer coupling depends on the interlayer electronic configuration. The proximity effect result in spin polarization of the graphene orbital by up to 63.6% together with a miniband splitting of about 73.4 meV and 8% notable enhancement in the magnetic moment (3.47 μ_B per cell) in the heterostructure. The position of the Dirac cone at Fermi level is strongly dependent on the graphene–$CrBr_3$ interlayer separation of 3.77 Å. Consequently, we also show that a perpendicular electric field can be used to control the miniband spin splitting and transmission spectrum. Also, the interfacial polarization effect due to the existence of two different constituents reinforces the conductivity via electrostatic screening in the heterolayer. These findings point towards the application potential of this unique system in nanoscale devices, where the electric field-driven magnetic proximity effect can lead to spin controllability and possible engineering of spin-gating.

(b) Combining DFT simulation with Wannier tight-binding approach makes it favourable to realize non-trivial topological properties and valley contrasting quantum anomalous Hall effect in proximitized Gr-$CrBr_3$ heterostructure with implications of relativistic effect. The valley contrasting QAH effect is observed with a nonzero Chern number at a high-symmetry point stemming from Berry curvature and Wannier charge center (WCC), leading to a topologically nontrivial state. The occurrence of strong magnetic proximity coupling between graphene and $CrBr_3$ monolayer is realized intrinsically, from shifting of Hall coefficient value near Fermi level. The opening of the global band gap (178 meV) is observed with the inclusion of spin orbit coupling (SOC). The anomalous Hall conductivity (AHC) demonstrates the presence of two maxima peaked at valley K′ and K. The observation of AHC is mainly dominated by nonzero surface charge and localized potential at the heterointerface due to proximity interaction. The Fermi level is found to be located exactly inside the nontrivial global band gap, which can be tuned effectively by applying the external electric field or by introducing a staggered sublattice potential. This robustness makes experimental fabrication highly beneficial for developing a valley contrasting QAH device prototype.

(c) The coexistence of longitudinal and transverse thermoelectric behaviour of magnetic proximity coupled has been investigated under the framework of First-principle based simulation and employed constant relaxation time approximation (CRTA). The asymmetric electronic structure near Fermi energy region is observed due to seamless proximity integration, depicting semimetallic-semiconductor characteristic. The asymmetric electronic behaviour contributes to the enhancement of Seebeck coefficient value, which contradicts the apprehensions of semimetal to be poor thermoelectric material. The electronic figure of merit supports the heterostructure system to be an ideal thermoelectric material. Moreover, the heterostructure is also flexible towards anomalous Nernst effect (transverse thermoelectric) with distinct oscillatory nature. The Seebeck and anomalous Nernst effect (ANE) shows high degree of tunability with applied external electric field. The synergistic existence of Seebeck and ANE due to proximity integration in vdW atomic crystal at room temperature will provide realistic approach to experimentally fabricate and develop real-time thermopower devices.

(d) Electric-field mediated spin-related phenomena together with magnetic proximity effect (MPE) en-routes new physical paradigm in developing nanoscale devices by modulating the functionalities of the materials. By employing first-principles calculation, we investigate MPE in a van der Waals (vdW) heterostructure constituted by a monolayer Weyl semimetal 1T′-WTe_2 (tungsten di-telluride), coupled with a monolayer ferromagnet $CrBr_3$ (chromium tribromide) at an interplanar distance of 3.68 Å. The proximity effect infers that the heterostructure system is 100% spin-polarized, with a spin-splitting of 25 and 10 meV for two spin configurations, leading to half-metallic nature. This robustness of MPE arises due to orbital hybridization and charge transfer at the interface of heterostructure system. Moreover, half-metallic nature is tuned and transformed to semiconducting and overlapping states in presence of external bias. The spin-splitting manifests orbital hybridization due to d-orbitals of W and Cr with a notable enhancement of 4% in the magnetic moment value (12.04 μB per cell). We also observe that proximitized interface is highly sensitive towards an application of external electric field. With external bias, the Fermi level across charge neutrality point is easily tuned and controls charge transport at interface. The consistent nature of conductivity enables the interfacial polarization and coherent electron drift is realized due to seamless proximity interaction across the transport channel of the heterostructure system. This electric field-mediated MPE in vdW heterostructure can strongly recommend for next-generation spin filtering and field effect transistor (FET) devices.

7.2 Future prospects

The inferences of the current thesis and its research outcome prompt to reconnoitre few fascinating aspects and designate new research predicament in near future. The following points mentioned below can be considered for future directions in the research field.

(i) Fluctuation of spins in 2D atomic crystals can be achieved by considering four basic Hamiltonians-Ising, Heisenberg, XY, Kitaev models-with respect to number of layers creating an interface for magnetic anisotropy energy and phase transition in strongly correlated electron system, which possibly aims to understand magnetic exciton, magnetic storage devices and spin-valley coupling.

(ii) Proximity effect can be extended by creating an interface by twisting the adjacent layers with a certain angle realizing Moire pattern in vdW atomic crystals for electronic and topologically non-trivial phases.

(iii) States like Majorana bound states in 2D proximitized quantum systems can be realized using density functional perturbation theory (DFPT) for realization of superconductivity.

(iv) Behaviour like magnetic skyrmions, i.e., topologically protected materials, which represent swirling spin-textures and chiral domain walls can show efficiency in room temperature devices.

(v) Quantum Monte Carlo (QMC) should be implemented for understanding the collective magnetic behaviour and interparticle interaction (exchange interaction, dipolar interaction etc.) in vdW quantum materials for tunnelling behaviour.

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