Appendix A

Methods and supporting information

A.1. Non-equilibrium Green's function (NEGF) formalism

The NEGF approach is one of the most powerful computation tools to evaluate the dynamical methods under the framework of non-equilibrium many-body systems. The NEGF formalism basically rules around the notion of quantum field theory to manage problems in statistical physics. The Poisson-Schrodinger equation has been solved self-consistently in case of NEGF formalism. Consequently, the expectation values of observables and correlation function can be provoked suitably by defining Green functions [1-3]. The NEGF method also has been used as a tool to computationally simulate transport properties of electrons in low-dimensional materials and its feasibility in designing nanoscale devices (shown in figure A. 1). This approach is incorporated in many software packages with different levels of sophistications such as combined with *ab initio*-based calculations [4] or constructs on effective physical model [5]. Figure A.1 represents the device prototype containing two leads (left and right), where middle region (scattering) is considered as dynamical one that governs tunnelling or transport of electrons of complete device. The two lead acts as the source and sink of charge carriers. Thus, the scattering region plays major role as it reacts with environment with the help of leads [6]. In chapter 3, we consider the ballistic transport mechanism via NEGF formalism in Gr-CrBr3 heterostructure system for which schematic figure shown in figure A.1.

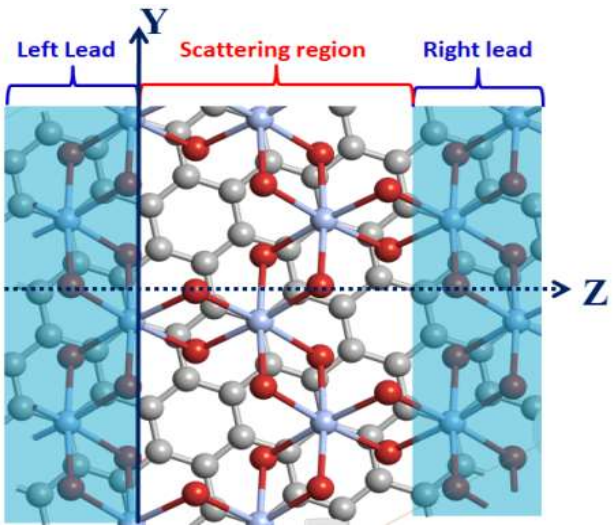

Figure A.1: Schematic illustration of a device prototype consisting three regions left lead, scattering region and right lead.

It is important to explore the quantum transport phenomena of charge carriers governing the quality of nanoscale devices. In this regard, it is necessary to build an effective theoretical approach and robust computational tool to investigate detail role of quantum transport phenomena of charge carriers in low-dimensional materials for efficient device performance. Therefore, implementing such tool helps in better clarity of exploiting the advances in scaling down to lower limit [7]. This also sets the stage for developing novel device and expects alternate fabrication techniques.

A.2. Interfacial Polarization

Van der Waals 2D heterostructure consists of heterogeneous mixtures of two or more constituents. In this structure, electric field polarization (known as the Maxwell-Wagner-Sillars effect) [8] occurs in the interface of the heterostructure system. Thus, the externally applied electric field generates charge which is distributed over the interface of the heterostructure system and migrates at interface forming large dipoles. These induced dipoles exhibit enhanced inertia and require sufficient time (low field frequency) and thermal agitation to follow the alternation of the applied electric field.

The theoretical analysis of the phenomenon leads to a dipolar effect with an additional term regarding the possible contribution of the charges to the overall conductivity of the system. Interfacial polarization can be described by the equations [4]:

$$\varepsilon^{'}(\omega) = \varepsilon_{\infty} + \frac{\varepsilon_s - \varepsilon_{\infty}}{1+\omega^2\tau^2} \quad \text{(A1)}$$

$$\varepsilon^{''}(\omega) = \frac{(\varepsilon_s - \varepsilon_{\infty})\omega\tau}{1+\omega^2\tau^2} \quad \text{(A2)}$$

where ε_s, ε_{∞} are the values of the real part of permittivity at low and high frequencies, σ the conductivity of the system, τ the relaxation time, ω the angular frequency of the applied electric field, and ε_0 the dielectric permittivity of free space (i.e., the interplanar spacing). Parameters ε_s, ε_{∞}, and σ are functions of the constituents' permittivity (ε_i), conductivity (σ_i), and volume fraction (v_i) and are given by the relations:

$$\varepsilon_s = \frac{\sum_i \frac{v_i \varepsilon_i^{'}}{\sigma_i^2}}{\sum_i (\frac{v_i}{\sigma_i})^2} \quad \text{(A3)}$$

$$\varepsilon_{\infty} = \frac{1}{\sum_i (\frac{v_i}{\varepsilon_i^{'}})} \quad \text{(A4)}$$

$$\sigma = \frac{1}{\sum_i (\frac{v_i}{\sigma_i})} \quad \text{(A5)}$$

Interfacial polarization is present in 2D heterostructure, especially in the case of a conductive reinforcing phase because of the coexistence of heterogeneous interfaces and stable crystalline phases [5]. The dramatic increase in interfacial area in heterostructures sets interfacial polarization as a predominant physical effect for their electrical performance.

A.3. Electronic thermal conductivity

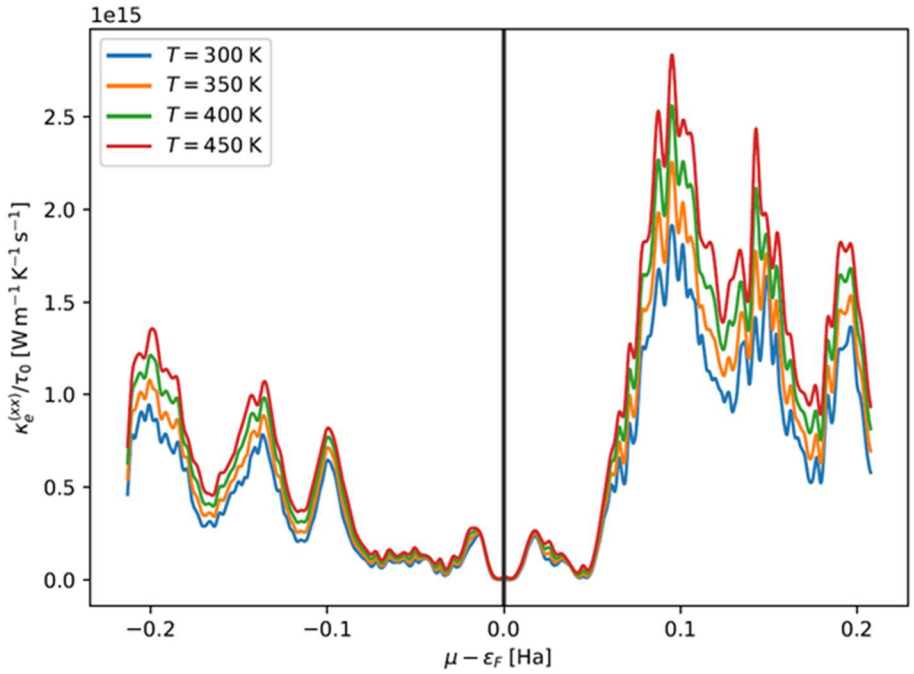

Figure A.2. The chemical potential dependent electronic thermal conductivity is measured for Gr-$CrBr_3$ vdW heterostructure at different temperatures from 300-450 K.

Figure A2 depicts electronic thermal conductivity with respect to chemical potential at temperature varied from 300 K to 450 K. The electronic thermal conductivity follows the same trend as electrical conductivity. The conductivity in n-type region is higher compared to p-type region corroborates well with electrical conductivity shown in figure. 5. 4(b). As the temperature increases, the thermal conductivity also increases as compared to room temperature. This is due to increase in kinetic energy of electrons and ultimately the collision of electrons occurs rapidly at interface, which increases thermal conductivity. The trend of electronic thermal conductivity justifies the heterostructure system to be an ideal thermoelectric material.

A.4. Electric field modulation of band topology in Weyl semimetal and ferromagnetic $CrBr_3$ vdW heterostructure

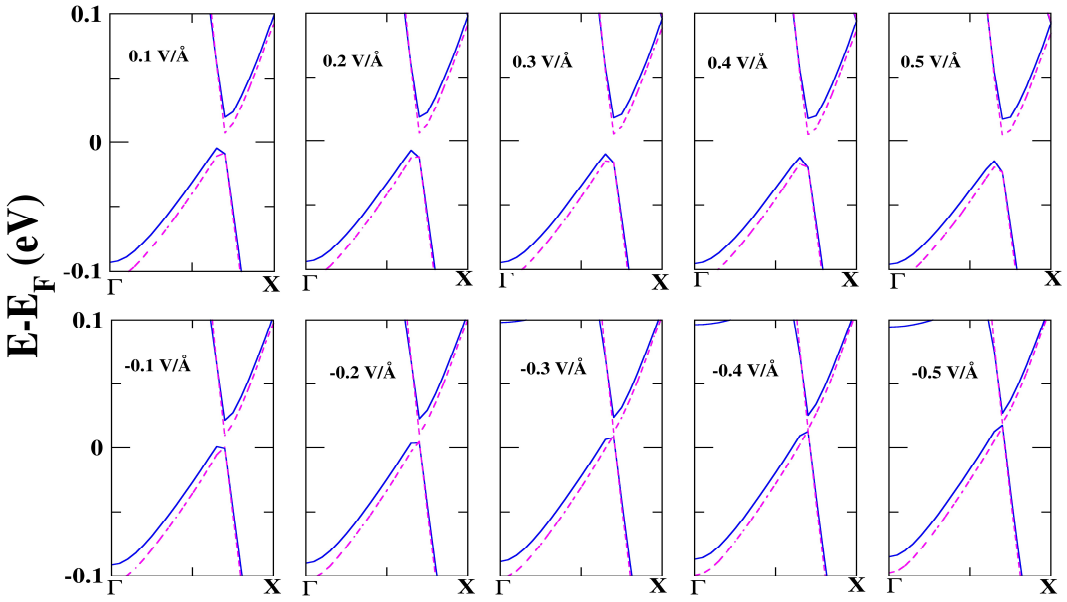

Figure A.3. The variation in band topology of vdW heterolayer system (1T'-WTe_2/$CrBr_3$) both forward and reverse (±0.5 V/Å) biasing along Z-direction. The blue continuous line represent spin-up states whereas magenta dashed line represent spin-down states, respectively.

Figure A3 depicts the tunability of band topology with respect to external bias in $\pm Z$-directions. With positive bias, the energy gap opens and at negative bias, the energy gap closes leading to interlayer polarization effect. This characteristic alteration in band topology can also utters the signature of switching ability making it feasible for DG-FET as well as field-effect switching applications.

A.5. Electrostatic potential of monolayer Weyl semimetal and ferromagnetic $CrBr_3$

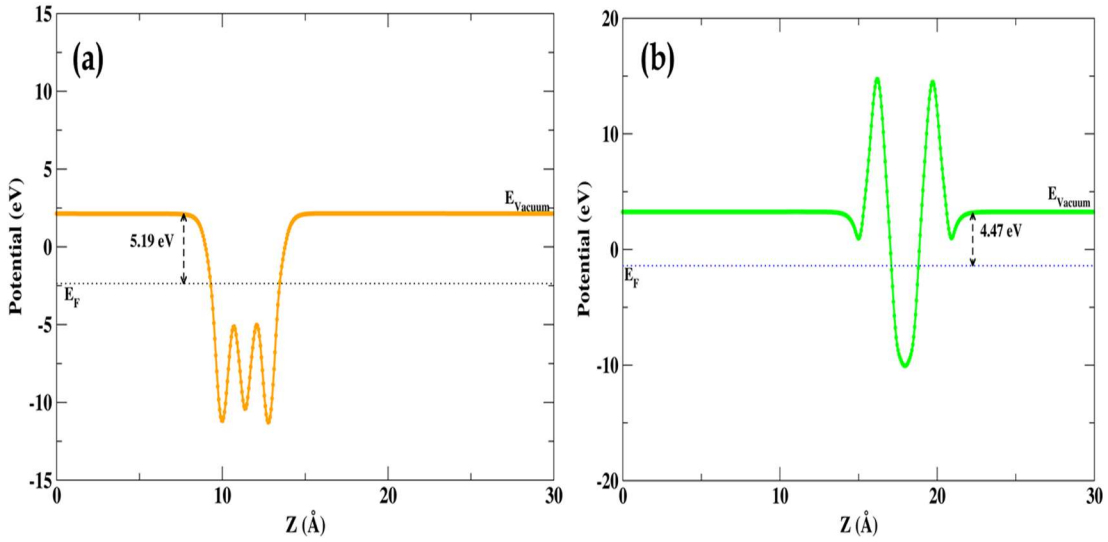

Figure A.4. Electrostatic potential curve of isolated $CrBr_3$ and isolated 1T′-WTe_2 layer along the Z-direction.

Figure A4 (a) and (b) depicts the electrostatic potential curve for isolated $CrBr_3$ and 1T′-WTe_2 layer along the Z-direction. The work function of isolated $CrBr_3$ layer is 5.19 eV which is near to the reported literature [11]. The work function of monolayer 1T′-WTe_2 is 4.47 eV which is in good agreement with the reported literature [12]. The isolated $CrBr_3$ layer has high electron affinity whereas isolated 1T′-WTe_2 has lower work function than $CrBr_3$. In this regard, while forming heterojunction $CrBr_3$ can accept electrons and WTe_2 will deplete the electrons. The transfer of electron will occur from monolayer Weyl semimetal (WSM) to ferromagnetic $CrBr_3$.

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Appendix B

Publications

B.1. List of publications

Articles published in peer-reviewed journals (included in thesis)

(a) **Bora, M.,** Mohanty, S., Singh, A. K., Gao, W. and Deb, P. Adaptive Half-metallicity via magnetic proximity in an electrically sensitive 1T'-WTe_2/$CrBr_3$ vdW heterostructure. *Applied Surface Science*, 623:157019, **2023**.

(b) **Bora, M.,** and Deb, P. Proximity induced longitudinal and transverse thermoelectric response in graphene-ferromagnetic $CrBr_3$ vdW heterostructure. *Journal of Physics: Condensed Matter*, 35:055402, **2023.**

(c) **Bora, M.,** and Deb, P. Density functional theory in two-dimensional Quantum materials. *Indian Journal of Theoretical Physics*, 70(1,2):7, **2022.**

(d) **Bora, M.,** Behera, S. K., Samal, P., and Deb, P. Magnetic proximity induced valley-contrasting quantum anomalous Hall effect in a graphene-$CrBr_3$ van der Waals heterostructure. *Physical Review B*, 105:235422, **2022.**

(e) **Bora, M.,** and Deb, P. Magnetic proximity effect in two-dimensional van der Waals heterostructure. *Journal of Physics: Materials*, 4:034014, **2021**.

(f) Behera, S. K*., **Bora, M*.,** Chowdhury, S. S. P., and Deb, P. Proximity effects in graphene and ferromagnetic $CrBr_3$ van der Waals heterostructure. *Physical Chemistry Chemical Physics*, 21:25788, **2019.** (*Authors contribute equally).

Articles (outside thesis)

(a) Das, J., **Bora, M.**, Deb, P., Ajayan, P. and Sahu, P. P. Redox mediated catalysis using β-FeNiCo-Hydroxide coated Superhydrophobic screw patch electrode in water splitting. (Communicated)

(b) Konwar, K., **Bora, M.,** Kaushik, S D., Chaturvedi, A., Kumar, D., Dutta, A., Mukhopadhyay, R., Babu, P D., Sharma, P., Lodha, S., Sen, D., Ajayan, P. and Deb, P. Exchange field induced Magnetic Resonance transverse relaxivity in

inhomogeneous anisotropy energy landscape of nano-ensemble. (Under review)

(c) Konwar, K., **Bora, M.,** Kaushik, S D., Prajapat, C L., Chaturvedi, A., Kumar, D., Sharma, P., Lodha, S., Sen, D., Babu, P D., and Deb, P. Nonergodic Quantum phenomena in cluster spin-glass ensemble of two-dimensional nanoflakes and a disintegrated framework. (Communicated)

Conference Proceedings

(a) **Bora, M.,** Behera, S. K. and Deb, P. Dynamic coalescence and implosion of internal microbubbles in immobile droplet. *AIP conference proceedings*, 2265:030014, 2020.

B.2. Papers presented in National and International conferences

- Presented poster entitled "**Proximity induced spin injection in Semimetal on Magnetic Insulator based Two Dimensional heterostructure**" at Advanced Simulation technique (ASM) 2019 organized by Indian Institute of Technology Delhi, New Delhi.
- Attended Workshop on Characterization of Magnetic materials 2019, National Institute of Technology (NIT)-Nagaland, Dimapur, India jointly organized by UGC-DAE Consortium for Scientific Research Mumbai Centre and NIT Nagaland, Dimapur, held during 27-29 November 2019.
- Presented poster on 64th DAE Solid State Physics Symposium 2019, Indian Institute of Technology (IIT) Jodhpur, Jodhpur-342037, Rajasthan, India organized by Bhabha Atomic Research Centre (BARC), Mumbai, India, 18-22 December 2019.
- Presented poster entitled "**Magnetic proximity effect in two-dimensional van der Waals crystals**" at 1st Asia-Pacific conference on Condensed Matter Physics 2021 in Dec 1-3, 2021.

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