Supplementary Information

Sign flipping intrinsic anomalous hall conductivity with Berry curvature tunability in a half-metallic ferromagent $NbSe_2$-VSe_2 lateral heterostructure

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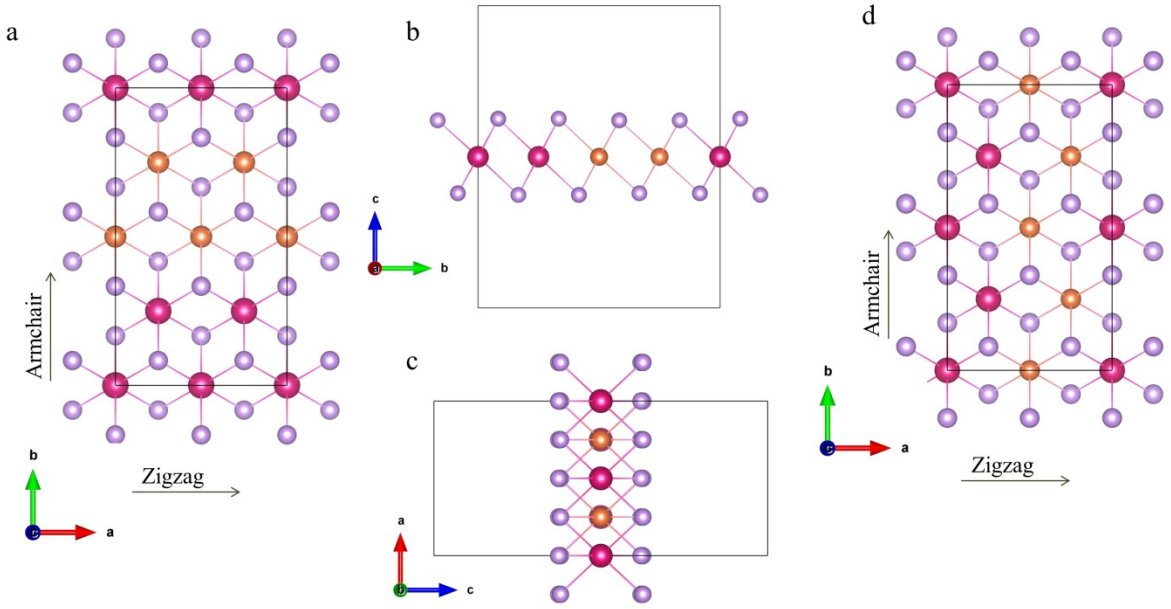

Figure S1: Figure: Geometric configuration of 2×2×1 zigzagged lateral heterostructure supercell along (a) top view (z-axis), (b) side view (along y-axis), (c) side view along x-axis and (d) top view of 2×2×1 supercell lateral heterostructure along armchair direction. Here, pink, orange and violet colour balls represent Niobium, Vanadium and Selenium atoms respectively.

The low formation energy of –0.57 eV of the system in zigzag direction over a value of -0.78 eV in armchair direction indicates that the heterointerface will naturally orient along zigzag direction. The formation energy ($E_{Formation}$), $E_{Formation} = (E_{HS} - E_{NbSe_2} - E_{VSe_2})/N$, is calculated using the above relation where, E_{HS} is the total energy of heterostructure in ziazag and armchair direction, E_{NbSe_2} and E_{VSe_2} are the energy of respective formula unit cell of $NbSe_2$ and VSe_2 monolayers. *N* is the total number of atoms in the supercell.

The calculated energy values are given below.

$E^{zigzag}{}_{HS} = -5222.14568354\ Ry$,

$E^{armchair}{}_{HS} = -5222.14019036\ Ry$

$E^{zigzag}{}_{NbSe_2} = -2850.67118172\ Ry$,

$E^{zigzag}{}_{VSe_2} = -2850.67118172\ Ry$,

$E^{armchair}{}_{NbSe_2} = -2850.59614974\ Ry$,

$E^{armchair}{}_{VSe_2} = -2370.16186457\ Ry$

Steps for making lateral heterostructure

1. Creating a two dimensional commensurate supercell of desired dimensions $n \times m \times 1$, where n, m are positive natural numbers with conditions that at least n and m or both being > 1 for a particular geometry. Here, we consider 2×2×1 supercell of 1T-$NbSe_2$ monolayer.

2. We replace Nb atoms with V atoms in the supercell either in zigzag or armchair orientations.

3. In this process, the distances and angles between Nb-Se and V-Se atoms have to be rearranged according to their respective 1T-$NbSe_2$ and 1T-VSe_2 unit cells, to retain original lattice constants.

4. After making the heterostructure, we optimize the system following self-consistency method as implemented in Quantum Espresso software for further electronic calculations.

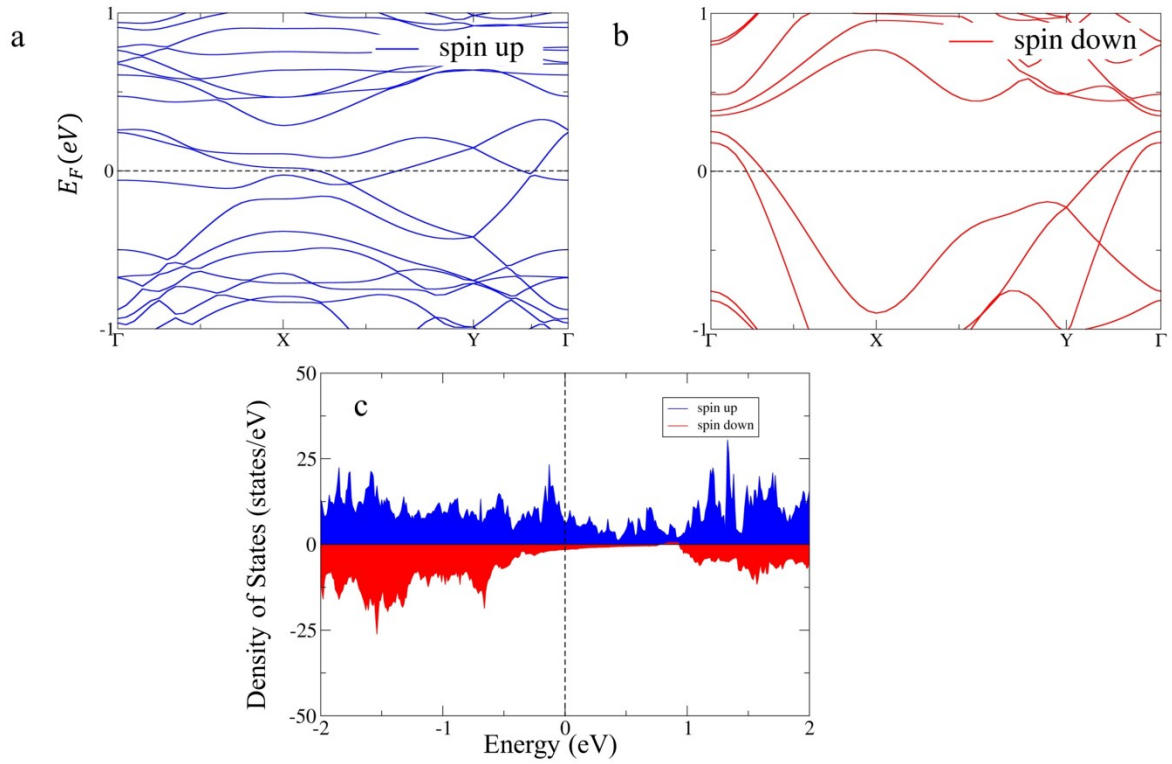

Figure S2: Band diagram (a-b) and Density of states plot for $NbSe_2$-VSe_2 lateral heterostructure in armchair direction.

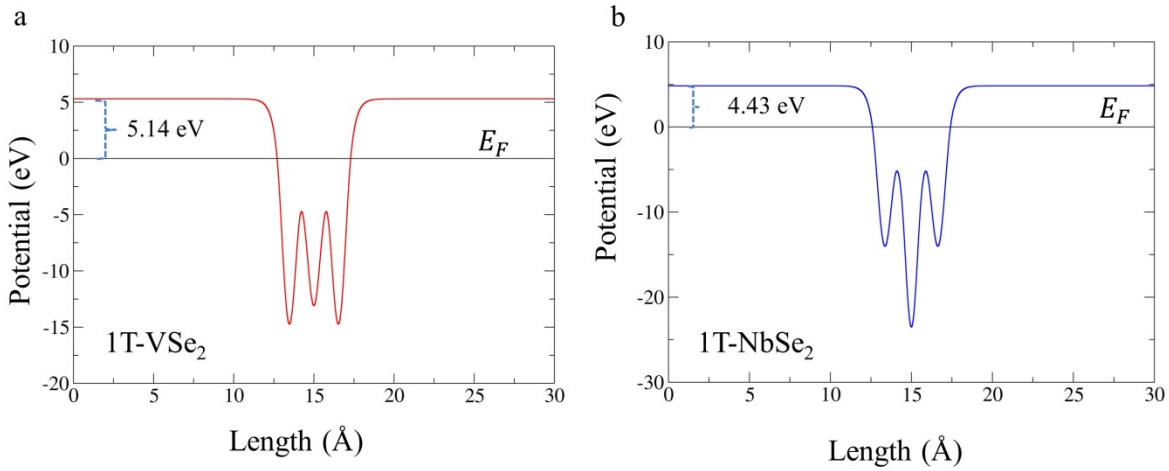

Figure S3: Illustration of Work function (WF) value for (a) 1T-VSe_2 and (b) 1T-$NbSe_2$ formula unit cells respectively.

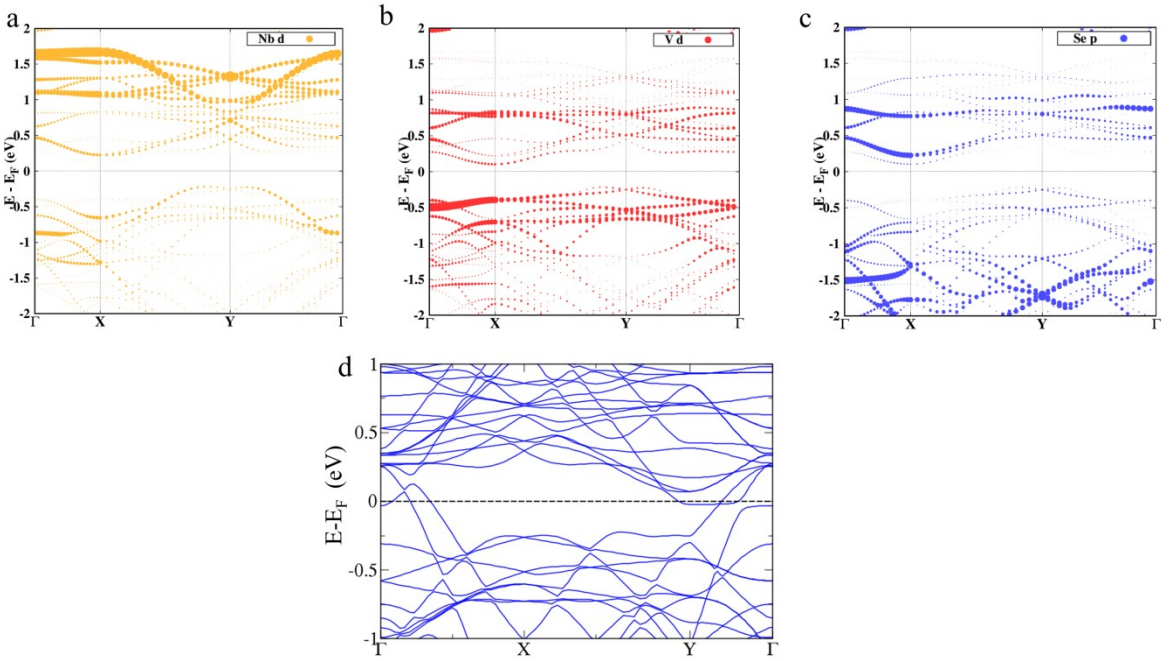

Figure S4: Orbital projected band diagram of 1T$NbSe_2$-1TVSe_2 lateral heterostructure. (a) Nb-d, (b) V-d , (c) Se-p orbital projected band diagram and (d) spin-orbit coupled (SOC) energy dispersion along $\Gamma - X - Y - \Gamma$ high symmetry path.

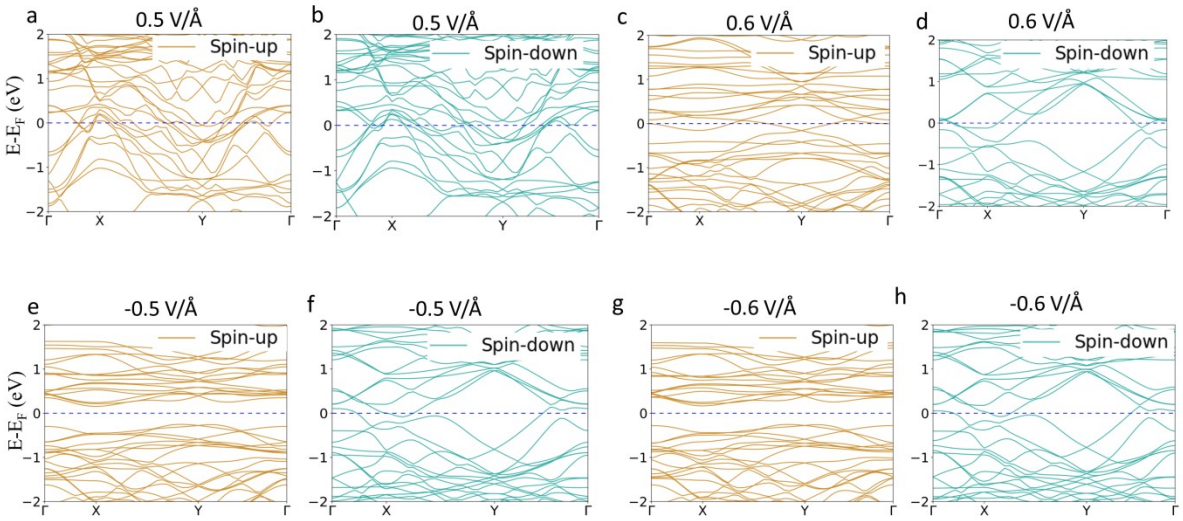

Figure S5: Energy band diagrams for spin and spin down electrons at electric field (a, b) 0.5 V/Å, (c, d) 0.6 V/Å, (e, f) -0.5 V/Å and (g, h) -0.6 V/Å.

The corresponding effect of half metal to metal transitions can be visualized in Figure S6, which represents the band structures of the lateral systems at electric field 0.5 V/Å and 0.6 V/Å. The band diagrams show clear evolution of no gapped states for the above two electric fields whereas the half metallic nature retains in reverse biasing directions. Owing to significant band crossing in metallic systems, it is expected to have reduced magnetic moments as it affects the spin polarization value of the system.

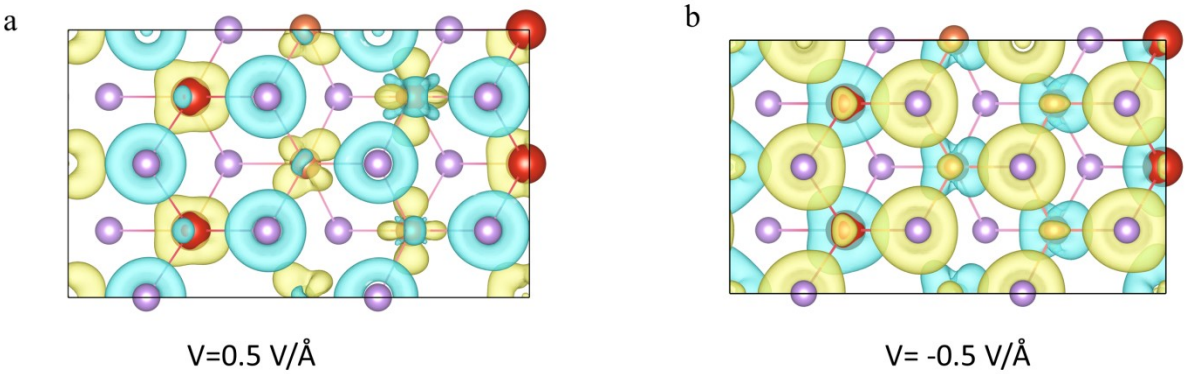

Figure S6: Charge redistribution under applied external electric fields at (a) V= 0.5 V/Å and (b) V = -0.5 V/Å respectively. Yellow color: net charge accumulation, cyan color: net charge dissipation.

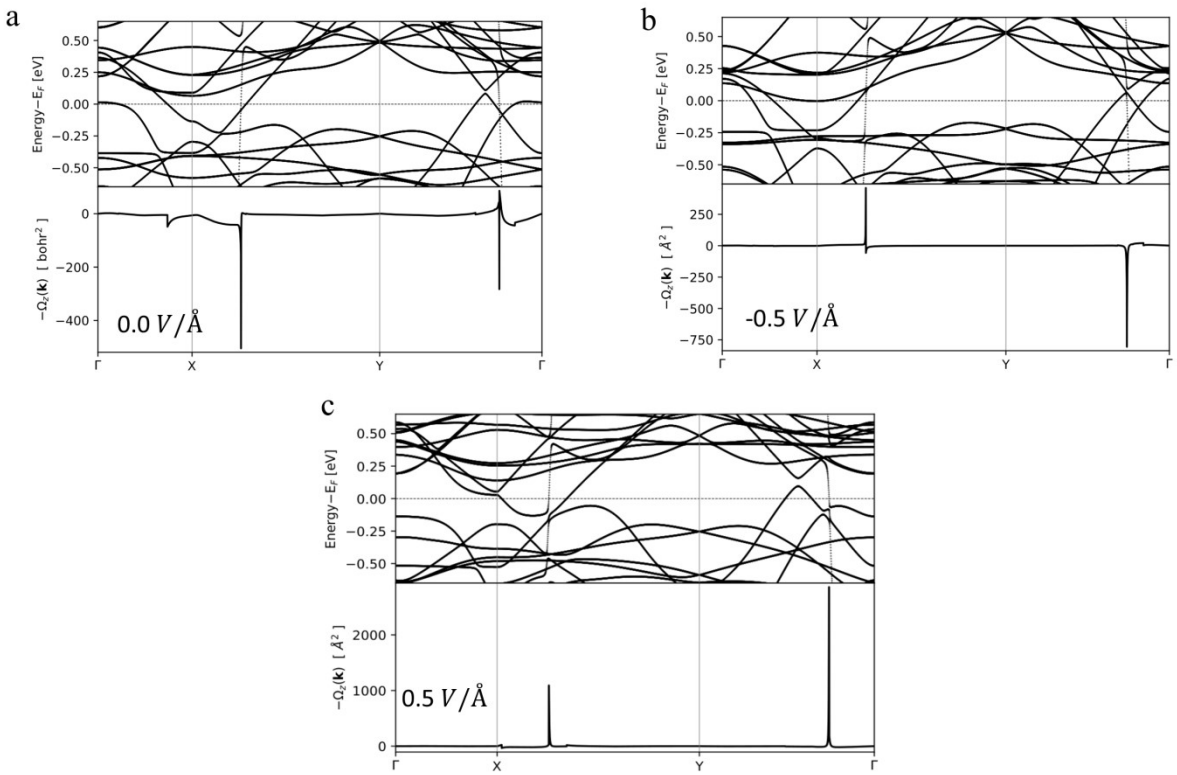

Figure S7: Spin-orbit coupling incorporated energy spectrum along with Berry curvatures at (a) $E = 0.0\, V/\text{Å}$, (b) $E = -0.5\, V/\text{Å}$ and (c) $E = +0.5\, V/\text{Å}$ along the high symmetry path $\Gamma - X - Y - \Gamma$.

Here, we present the calculation of Berry curvature together with energy band diagram along high symmetry points. The spread values for 176 number of Wannier bands with SOC at $\vec{E} = 0\, V/\text{Å}$, $-0.5\, V/\text{Å}$ and $+0.5\, V/\text{Å}$ are 755.737001374 Å^2, 610.134239914 Å^2 and 556.257375675 Å^2 respectively.

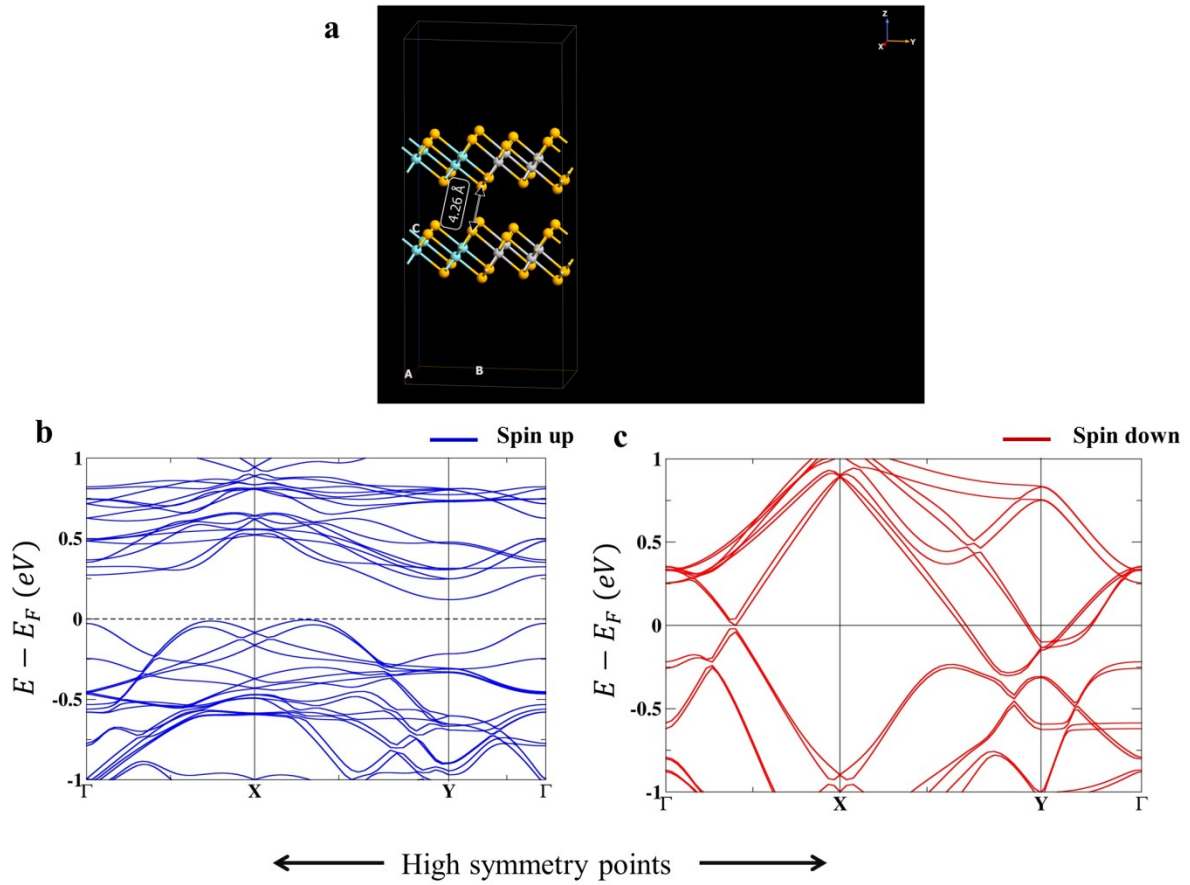

Figure S8: (a) Optimized bilayer geometric configuration at an interlayer separation 0f 4.26 Å, Spin polarized energy band diagram for bilayer $NbSe_2$-VSe_2 lateral heterostructure for (b) Spin up (blue) and (c) Spin down (red) electron channels. Blue and red color represents spin up and down orientation of electrons in the material. (Color Balls: Blue- Nb atom, Silver -V atom and Yellow- Se atom)

We plot the electronic band structure of the two layers $NbSe_2$-VSe_2 lateral heterostructure consisting 48 numbers of atoms in unit cell, with an optimized interlayer distance of 4.26 Å. We observe a gapped character for spin up channels while spin down channel remains conducting, similar to its single layer heterostructure. The spin polarized band diagram is provided below.

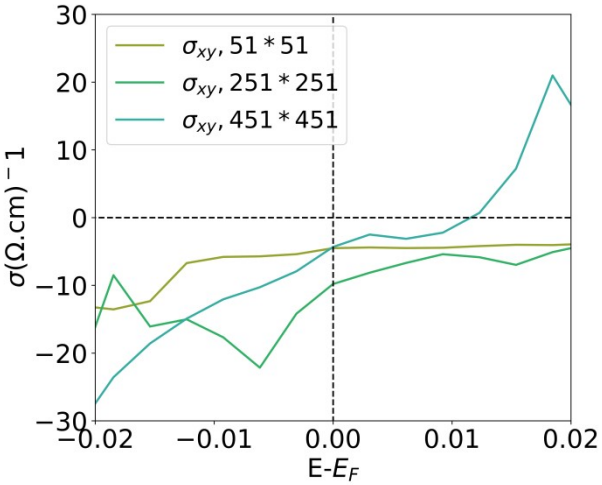

Figure S9: Obtained AHC value for different grid point set for zero bias system.

We observe that the AHC value at $51 \times 51 \times 1$, $251 \times 251 \times 1$ and $451 \times 451 \times 1$ are found to be -4.51 S/cm, -9.8 S/cm and -4.33 S/cm respectively. The AHC value at $651 \times 651 \times 1$ is found to be -5.2 S/cm. The calculated AHC values at different grid sets are within 1-2% error bar. Hence, we choose the dense grid sets for calculations of Berry related properties.