Supplementary Information

Berry Curvature Dipole-induced Non-linear Hall Effect in Oxide Superlattices

Nesta Benno Joseph,[a,*] Arka Bandyopadhyay,[b] Ajit C. Balram,[c,d] Awadhesh Narayan[a,$]

[a]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560012, India
[b]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany
[c]Institute of Mathematical Sciences, CIT Campus, Chennai 600113, India
[d]Homi Bhabha National Institute, Training School Complex, Anushaktinagar, Mumbai 400094, India
[*]nestajoseph@iisc.ac.in [$]awadhesh@iisc.ac.in

S1 Formation energy

To determine the thermodynamic stability of the superlattices, the formation energies (E^{form}) were calculated using the formula,

$$E^{\text{form}} = \frac{E_{SL} - n_A E_A^{\text{bulk}} - n_B E_B^{\text{bulk}}}{n_A + n_B}, \tag{1}$$

where E_{SL} is the energy of the superlattice, E_A/E_B is the energy of the bulk A/B system, and n_A/n_B is the number of layers of A/B in the superlattice. The bulk energies of $BaOsO_3$ and $BaIrO_3$ were calculated by starting with a cubic perovskite structure, and relaxing only the out-of-plane component, to keep the in-plane lattice constant consistent with BTO, and atomic coordinates. The formation energies, in units of meV/formula, of the systems were found to be as presented in Table S1.

Table S1 Formation energy associated with the four superlattices.

Superlattice	E_{form} (meV/f.u.)
$(BaOsO_3)_1/(BTO)_4$	-37.03
$(BaIrO_3)_1/(BTO)_4$	38.67
$(BaOsO_3)_2/(BTO)_4$	-59.83
$(BaIrO_3)_2/(BTO)_4$	-3.17

The formation energy per formula unit is negative, meaning these superlattices are thermodynamically stable, except for $(BaIrO_3)_1/(BTO)_4$. This value, however, is only approximately 38 meV/f.u. above formation threshold. Given that DFT calculated energies have errors which are larger than this value [1–3], the $(BaIrO_3)_1/(BTO)_4$ superlattice (and the other proposed structures) could very well be within the reach of experiments. Furthermore, $(BaIrO_3)_2/(BTO)_4$ has a small but negative formation energy. This suggests that superlattices with a larger number of $BaIrO_3$ layers tend to be more thermodynamically stable.

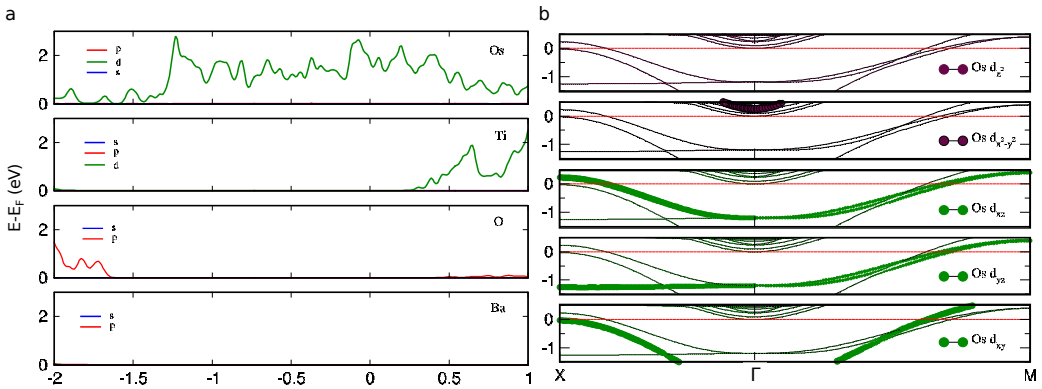

Fig. S1 (a) Projected density of states associated with Os, Ti, O and Ba atoms in $(BaOsO_3)_1/(BTO)_4$ superlattice. The red, green and blue indicate p, d and s states respectively. (b) Os d orbitals projected onto the band structure of $(BaOsO_3)_1/(BTO)_4$ superlattice. The solid green circles indicate d_{xy}, d_{yz} and d_{zx} states and solid maroon circles indicate d_{z^2} and $d_{x^2-y^2}$. The former three orbitals dominate the bands around Fermi level.

S2 Wannierization

The Wannier interpolation was done using O p, Ti d and Os/Ir d orbitals as the basis. Fig. S1 (a) shows projected density of states (DOS) of Ba, Ti, O and Os of $(BaOsO_3)_1/(BTO)_4$ superlattice. It can be seen that the metallicity arises due to the Os d states, especially the Os d_{xy}, d_{yz} and d_{zx} states as shown in Fig. S1 (b). This is true for the other superlattices as well.

The basis for the Wannier TB model was chosen using this information. Fig. S2 shows comparison of the band structures computed using both DFT and Wannier calculations for the four superlattices considered. It can be seen that the two band structures exaclty overlap, indicating that the TB model constructed accurately describe the superlattices under study.

S3 Variation of BCD with temperature

We used our Wannier-based TB Hamiltonian to compute the Berry curvature and associated BCD using the WANNIER-BERRI code. The Berry curvature and BCD calculations were done at a temperature of 40 K. Increasing this temperature broadens the features in the BCD as a function of the Fermi level, as shown in Fig. S3.

References

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[3] A. Narayan, A. Bhutani, S. Rubeck, J. N. Eckstein, D. P. Shoemaker and L. K. Wagner, *Physical Review B*, 2016, **94**, 045105.

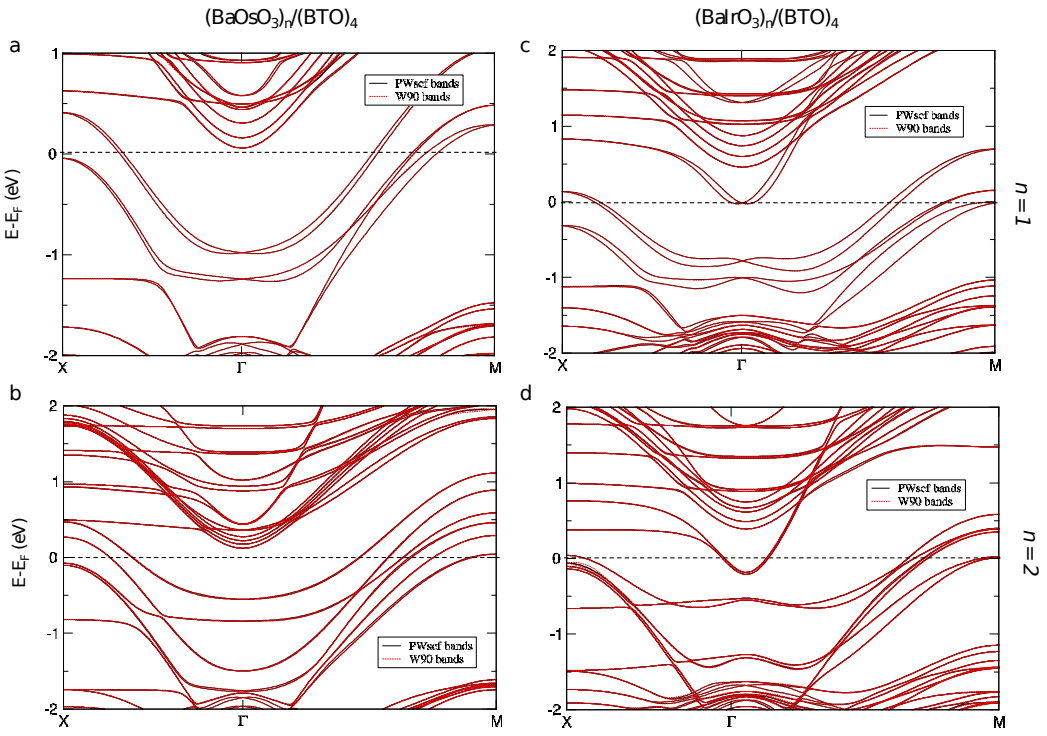

Fig. S2 Comparison of DFT (black solid) and Wannier bands (red dotted) for $n = 1$ and $n = 2$ heterostructures.

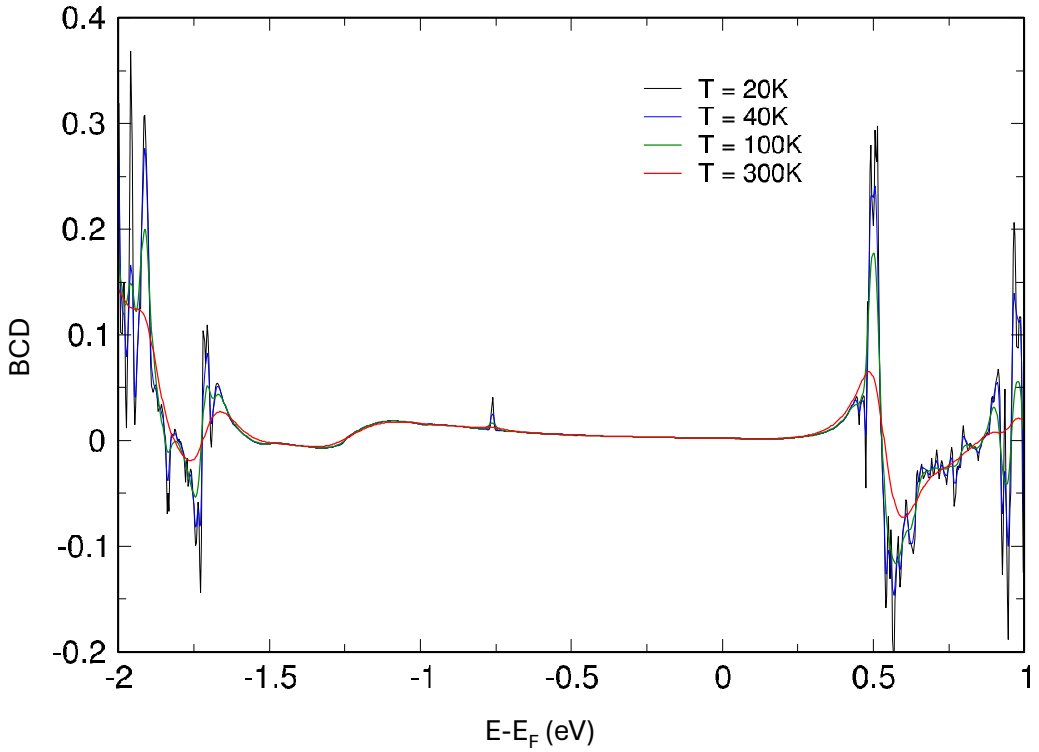

Fig. S3 The BCD component D_{xy} of $n = 1$ superlattice $(BaOsO_3)_1/(BTO)_4$ at different temperatures. The BCD as a function of the Fermi level broadens as a result of increasing temperature.