First-principles study on electronic properties in $BiFeO_3$ based heterostructures

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Abstract

The $BiFeO_3/SrTiO_3$(001) and $BiFeO_3/PbTiO_3$(001) heterostructures(HS) are investigated with two types of interfaces. Recently, using density functional theory (DFT) based first-principle calculations, evidence of half-metallicity is observed in a bulk tetragonal phase of $BiFeO_3$(TBFO). The same structure exhibits half-metallicity along with two-dimensional hole gas (2DHG) on the TBFO(001) surface as well.In this work, two types of TBFO based heterostructures are studied as mentioned above in order to examine the persistence of half-metallicity in these perovskite based heterostructure systems. In case of $BiFeO_3/SrTiO_3$(001) (TBFO/STO) HS the $(FeO_2)^-/(SrO)^0$, and $(BiO)^+/(TiO_2)^0$ interfaces are investigated respectively.For $BiFeO_3/PbTiO_3$(001) (TBFO/PTO) HS the $(FeO_2)^-/(PbO)^0$, and $(BiO)^+/(TiO_2)^0$ interfaces are studied. A tiny amount of half-metallicity(Hmfm) appeared in the $(FeO_2)^-/(SrO)^0$ interface while $(BiO)^+/(TiO_2)^0$ interface contributes to metallicity in case of TBFO/ STO interface.Interestingly, $(FeO_2)^-/(PbO)^0$ interface turns out to be a distinct half-metal with hole-type charge carriers and $(BiO)^+/(TiO_2)^0$ behave as two-dimensional electron gas (2DEG) in case of TBFO/PTO HS.

Structural and computational details

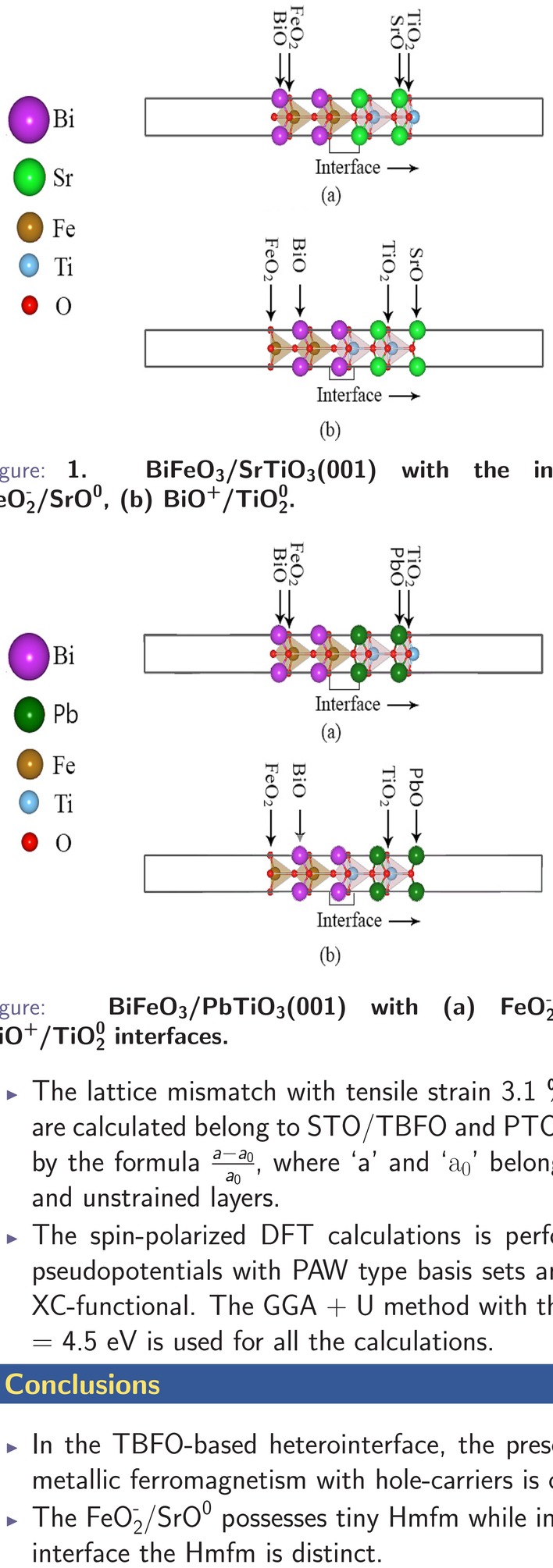

Figure: **BiFeO$_3$/SrTiO$_3$(001) with the interfaces (a) FeO$_2^-$/SrO^0, (b) BiO$^+$/TiO$_2^0$.**

Figure: **BiFeO$_3$/PbTiO$_3$(001) with (a) FeO$_2^-$/PbO^0, (b) BiO$^+$/TiO$_2^0$ interfaces.**

- The lattice mismatch with tensile strain 3.1 % and 3.6 % are calculated belong to STO/TBFO and PTO/TBFO HSs by the formula $\frac{a-a_0}{a_0}$, where 'a' and 'a_0' belong to strained and unstrained layers.
- The spin-polarized DFT calculations is performed. The pseudopotentials with PAW type basis sets and PBE type XC-functional. The GGA + U method with the value of U = 4.5 eV is used for all the calculations.

Conclusions

- In the TBFO-based heterointerface, the presence of half-metallic ferromagnetism with hole-carriers is observed.
- The FeO$_2^-$/SrO^0 possesses tiny Hmfm while in FeO$_2^-$/PbO^0 interface the Hmfm is distinct.
- In case of TBFO/PTO(001), the BiO$^+$/TiO$_2^0$ interface exhibits 2DEG.
- The heterostructures belong to FeO_2 based interface, turns out to be energetically more stable as compared to BiO based interface, which is observed to possess half-metallicity.

Results and Discussion

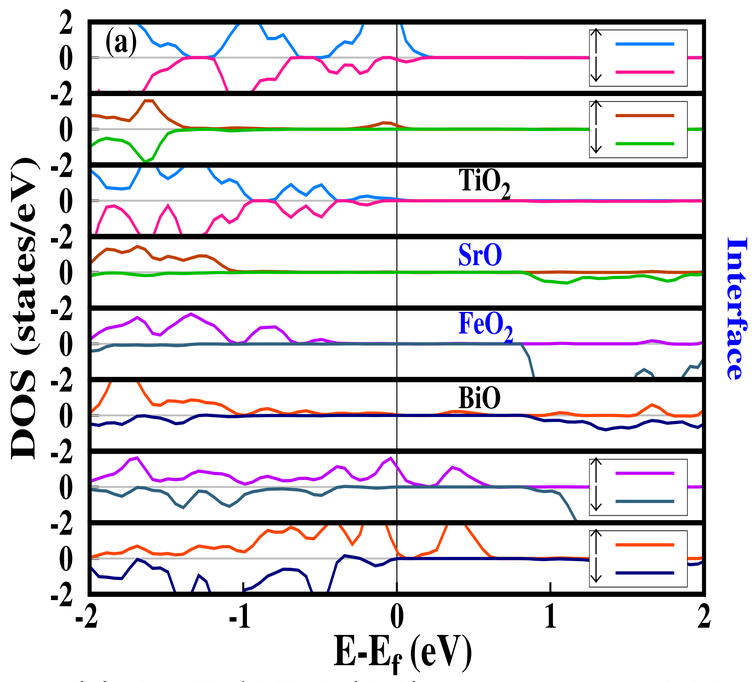

Figure: **(a) BiFeO$_3$/SrTiO$_3$(001): layer-resolved DOS of FeO$_2^-$/SrO^0 interface.**

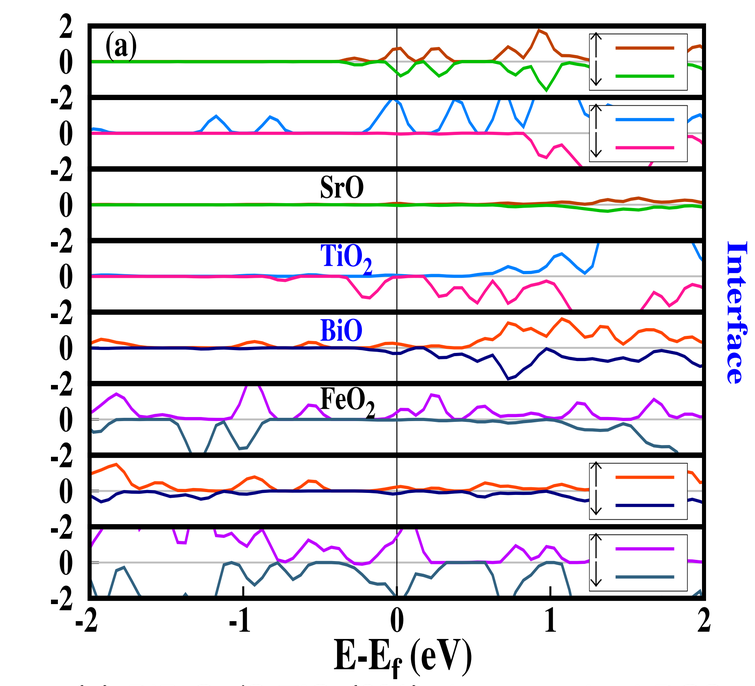

Figure: **(a) BiFeO$_3$/SrTiO$_3$(001): layer-resolved DOS of BiO$^+$/TiO$_2^0$ interface.**

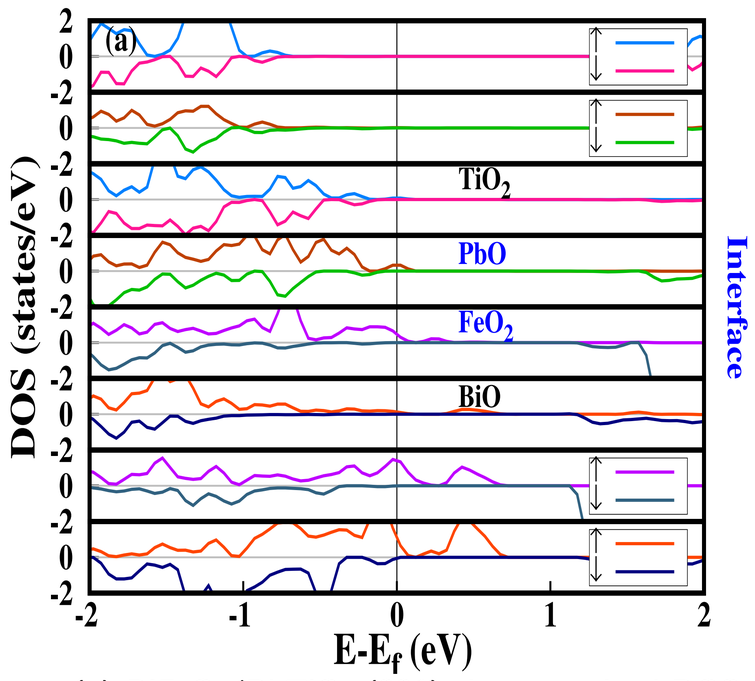

Figure: **(a) BiFeO$_3$/PbTiO$_3$ (001): layer-resolved DOS of FeO$_2^-$/PbO^0 interface.**

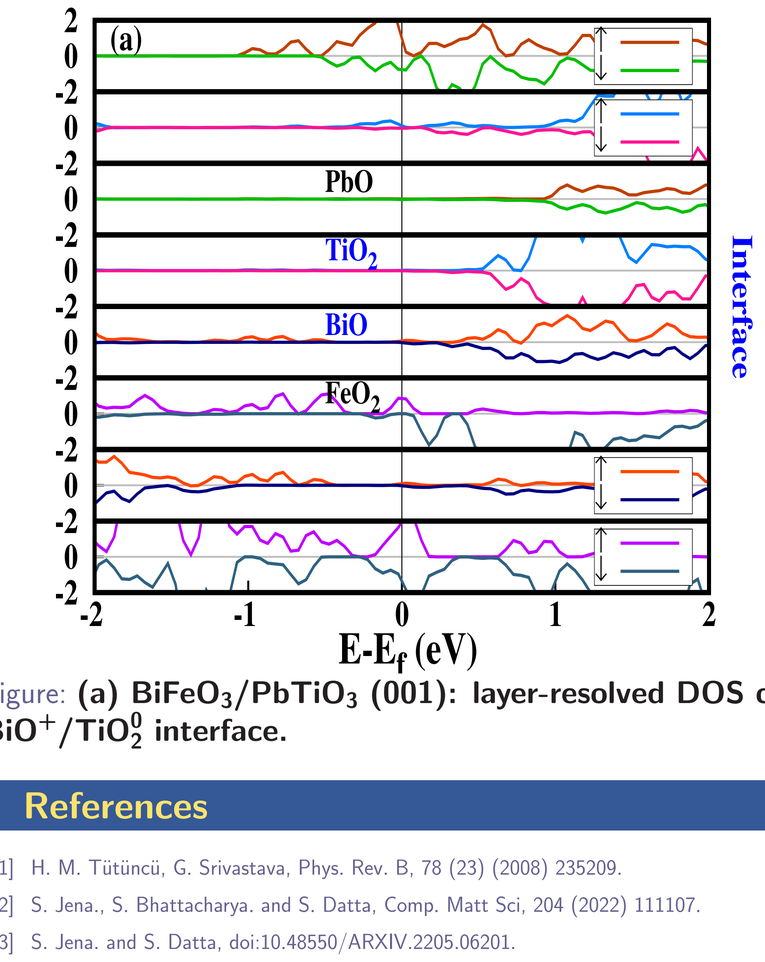

Figure: **(a) BiFeO$_3$/PbTiO$_3$ (001): layer-resolved DOS of BiO$^+$/TiO$_2^0$ interface.**

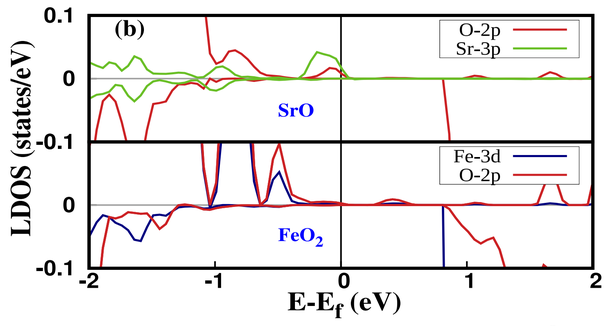

Figure: **(b) Local-DOS belong to FeO$_2^-$/SrO^0 interface.**

- A very tiny amount of half-metallic ferromagnetic (Hmfm) is spotted in this interface.
- The $Sr-3p$, $O-2p$,$Fe-3d$ orbital contributions are observed.
- From the PDOS analysis, $Sr-3p_x,p_y,p_z$ and $O-2p_z$ orbitals along with $Fe-3d-e_g$ and all the $O-3p_x,p_y,p_z$ orbital contributions are observed.

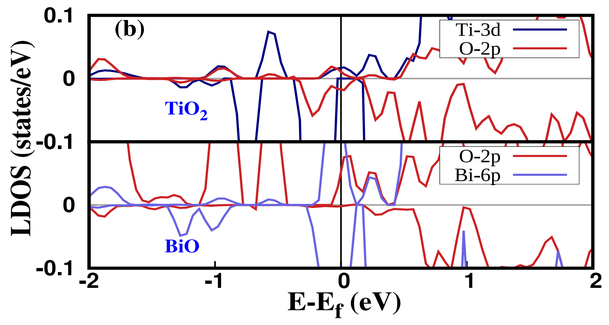

Figure: **(b) Local-DOS belong to BiO$^+$/TiO$_2^0$ interface.**

- This interface exhibits ferromagnetic metallicity.
- In addition, the $Ti-3d$, $O-2p$ and $Bi-2p$ orbital contributions are observed.
- From the PDOS analysis, measure contributions of $Ti-3d-e_g$ and $O-2p_z$ orbitals and $Bi-6p_x,p_y,p_z$ and $O-2p_x,p_y,p_z$ contributions are found.

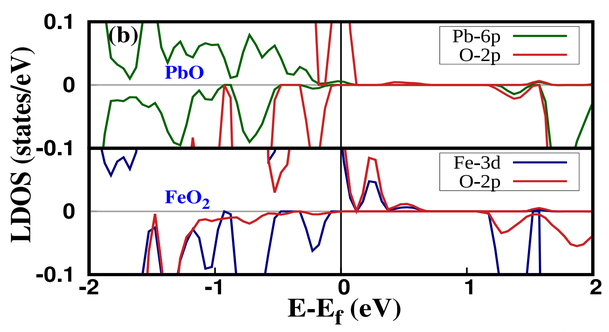

Figure: **(b) Local-DOS belong to FeO$_2^-$/PbO^0 interface.**

- In this case, distinct Hmfm state along with hole-carriers are observed.
- The contribution of $Pb-6p$, $O-2p$ and $Fe-3d$ orbitals are observed.
- From PDOS analysis, both $Fe-e_g$ and t_{2g} and $O-2p_x,p_y,p_z$ orbitals along with $Pb-6p_z$ and $O-2p_x$ and $2p_y$ are found to contribute to Hmfm.

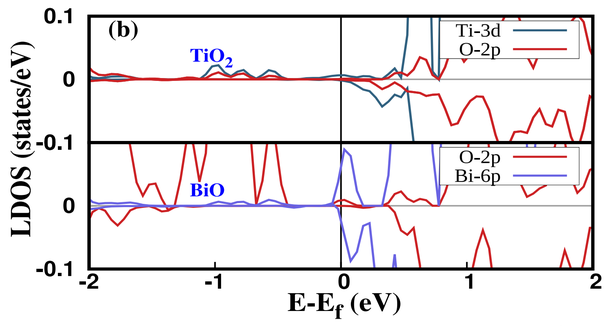

Figure: **(b) Local-DOS belong to BiO$^+$/TiO$_2^0$ interface.**

- In this case two-dimensional electron gas(2DEG) is observed in the interface from both the spin-channel.
- The contributions of $Ti-3d$, $O-2p$ and $Bi-6p$ orbitals are found.
- From PDOS analysis, the contribution of $Ti-e_g$ and $O-2p_z$ along with $Bi-6p_z$ and $O-2p_z$ are observed.

References

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