Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information(ESI) of ``Evidence of Half-metallicity at the $BiFeO_3$ (001) surface''

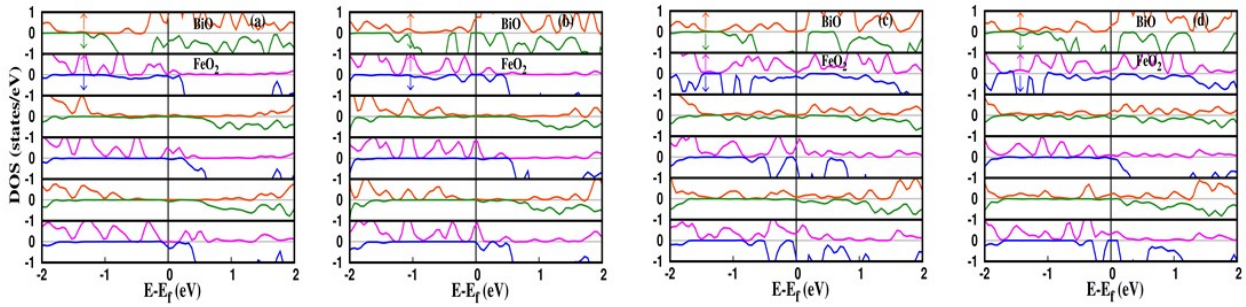

Fig. 1 Density of states (DOS) of 4L slab-thicknesses with BiO termination for (a) structure-I, (b) structure-II, (c) structure-III, and (d) structure-IV respectively.

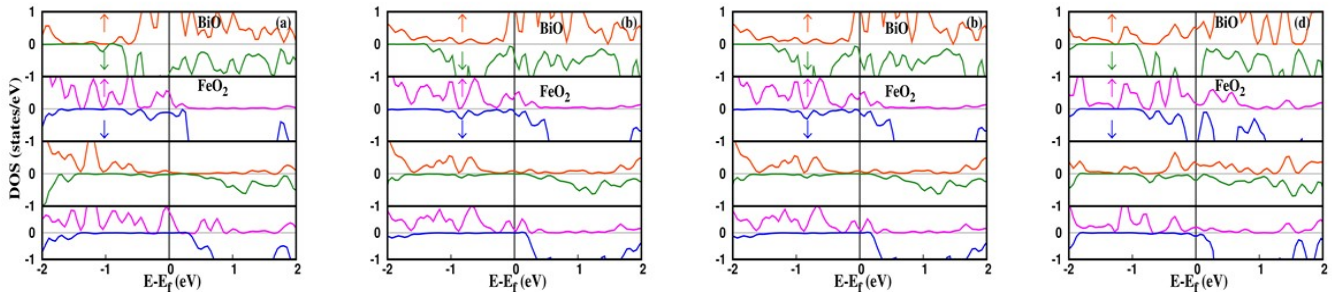

Fig. 2 Layered density of states (DOS) of 6L surface-thicknesses with BiO termination (a) structure-I, (b) structure-II, (c) structure-III, and (d) structure-IV respectively.

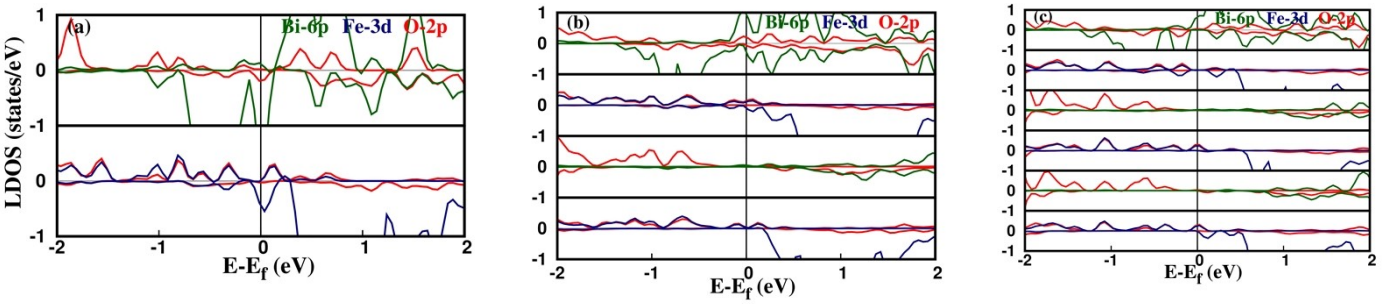

Fig. 3 Local density of states (LDOS) of structure-II with BiO terminated surface thickness of (a) 2L, (b) 4L and (c) 6L respectively.

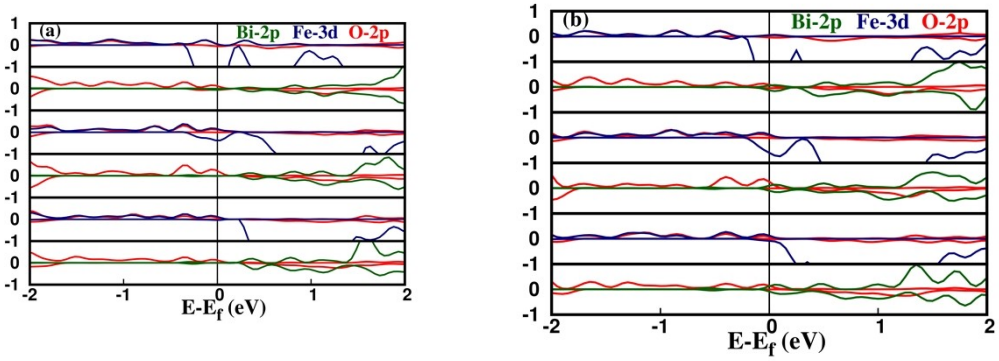

Fig. 4 Local density of states (LDOS) of 6L slab-thicknesses with FeO2 termination for (a) structure-III and (b) structure-IV respectively.