

Fig. 6 Layered density of states (DOS) corresponding to Structure-II with oxygen vacancy at 'V1' site on FeO₂ terminated surface thickness of (a) 2L, (b) 4L and (c) 6L respectively.

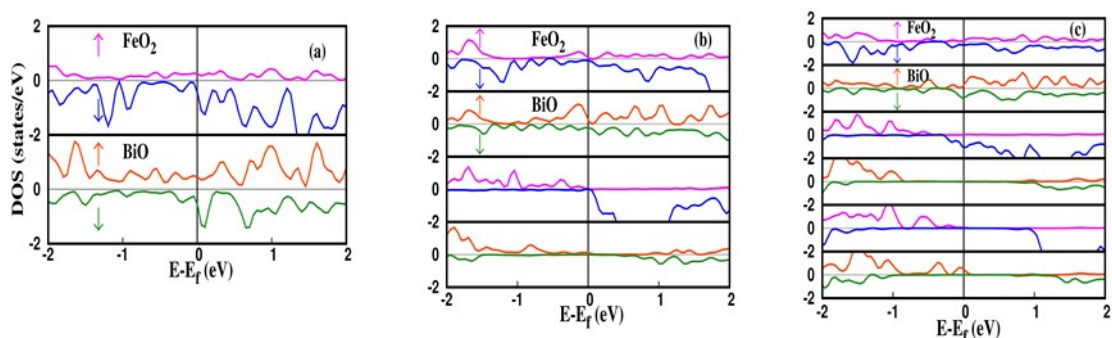


Fig. 7 Layered density of states (DOS) corresponding to Structure-II with oxygen vacancy at 'V2' site on FeO₂ terminated surface thickness of (a) 2L, (b) 4L and (c) 6L respectively.

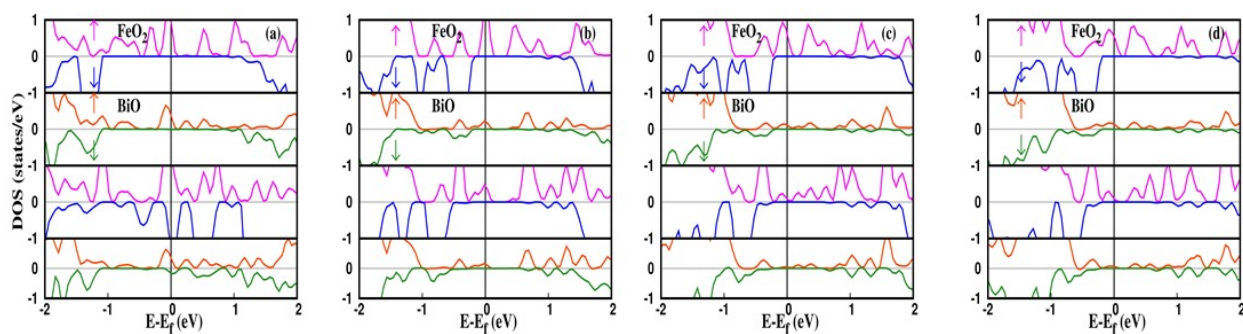


Fig. 8 Density of states (DOS) of 4L slab-thicknesses with FeO₂ termination for (a) structure-I, (b) structure-II, (c) structure-III, and (d) structure-IV respectively.

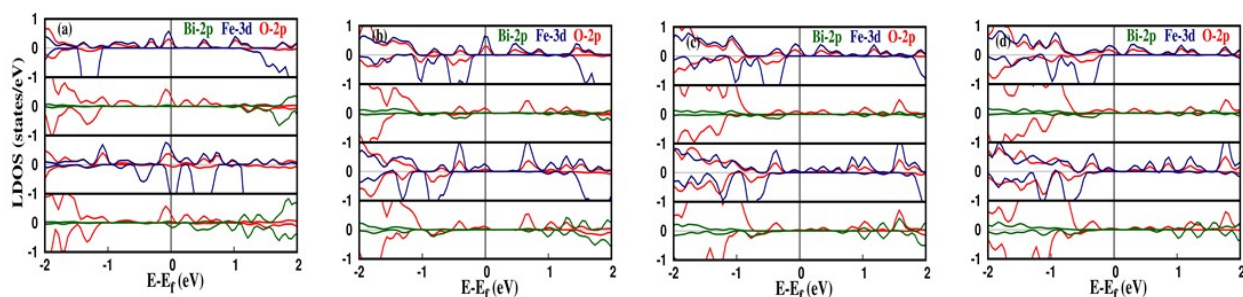


Fig. 9 Local density of states (LDOS) of 4L slab-thicknesses with FeO₂ termination for (a) structure-I, (b) structure-II, (c) structure-III, and (d) structure-IV respectively.