Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

Fig.S1. Top and side views of the geometric structures for Ni adatom adsorbs on Pt(111) supported PBG and DBG sheets. (a)-(b) H site of top and bottom layer (PBG) and (c)-(d) upper and below SV site (DBG), respectively. Black, gray and green balls represent C, Ni and Pt atoms, respectively.

Fig.S2. Spin-resolved TDOS and PDOS for (a)-(b) Ni and (c)-(d) Fe atom anchors on PBG (H site) and (b) DBG (below SV site) using PBE+U calculation. The solid lines represent the TDOS of PBG (or DBG) with the adsorbed Ni (or Fe) atom and dashed lines represent the PDOS of Ni (or Fe) *3d* states. The vertical dotted line denotes the Fermi level.

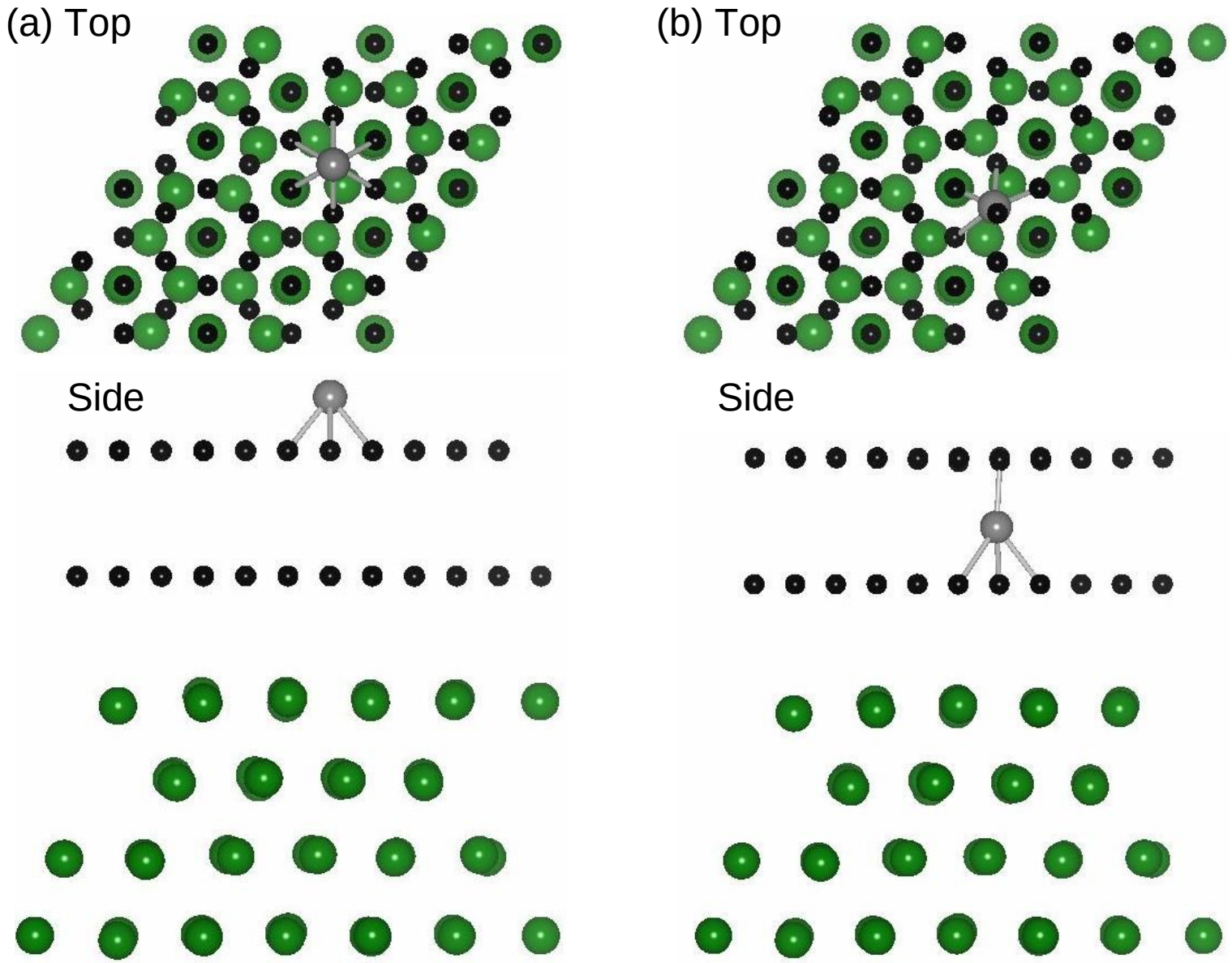

Fig. S1(a)-(b)

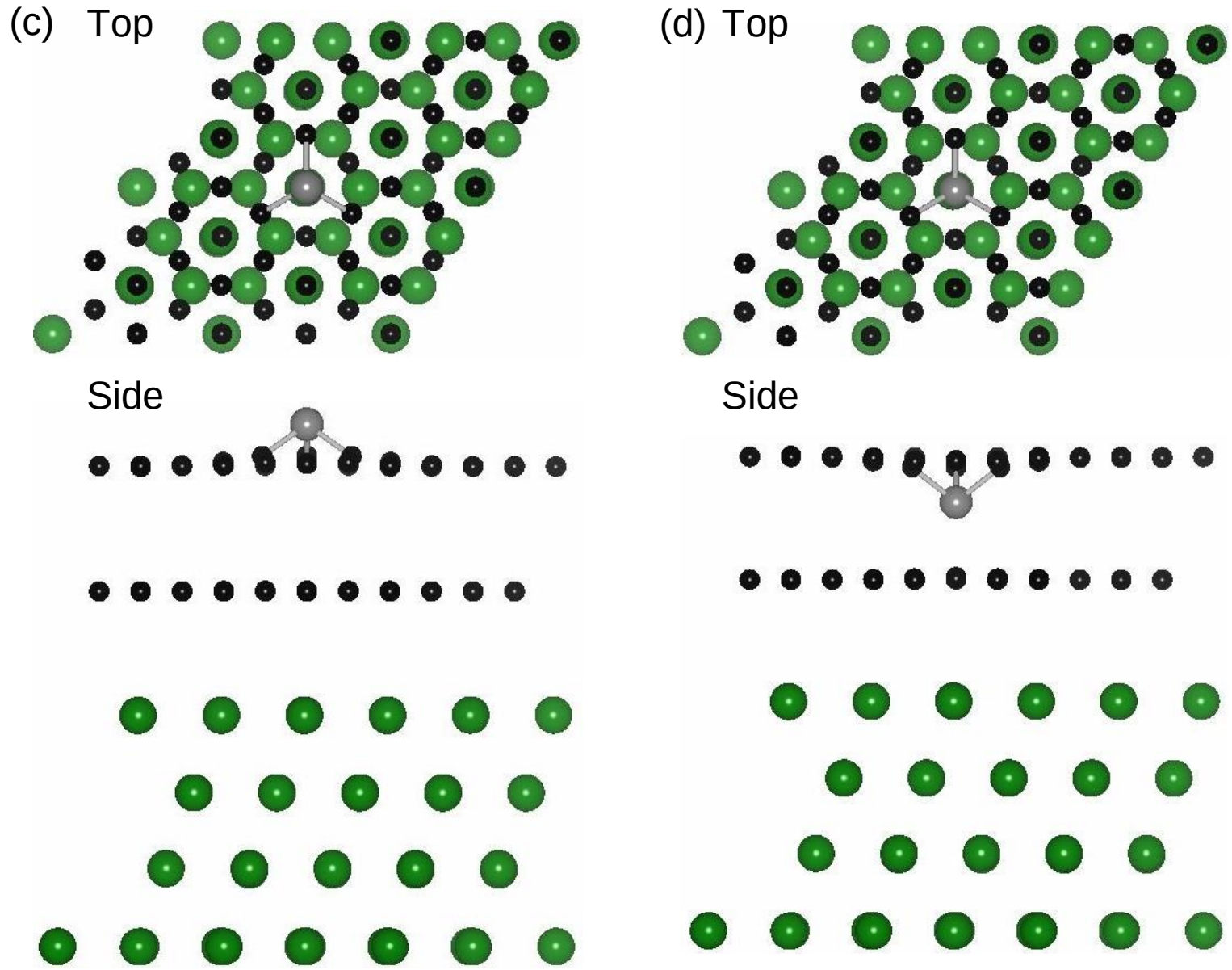

Fig. S1(c)-(d)

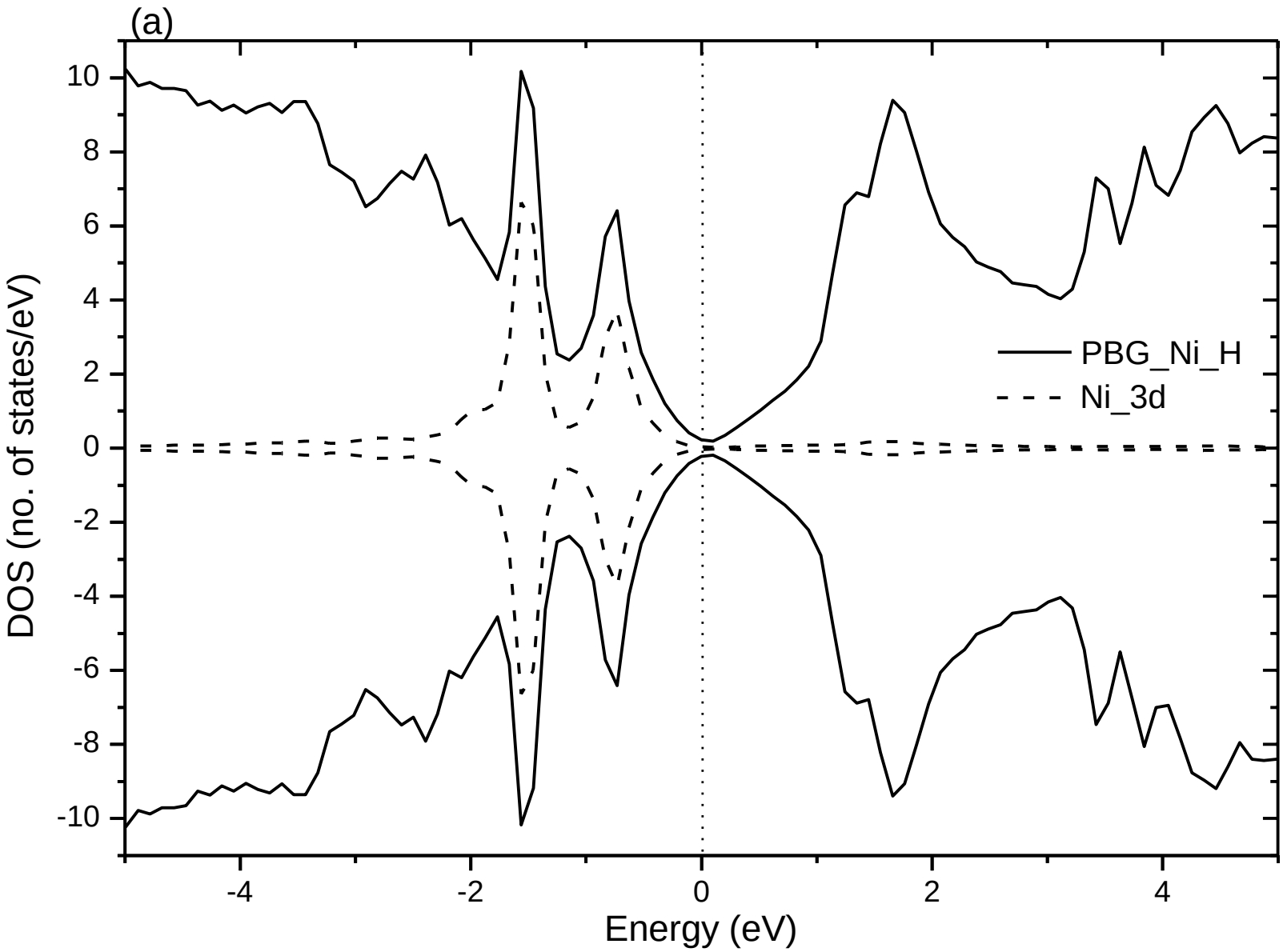
(a)
DOS (no. of states/eV)
Energy (eV)
PBG_Ni_H
Ni_3d
10
8
6
4
2
0
-2
-4
-6
-8
-10
-4
-2
0
2
4

Fig. S2(a)

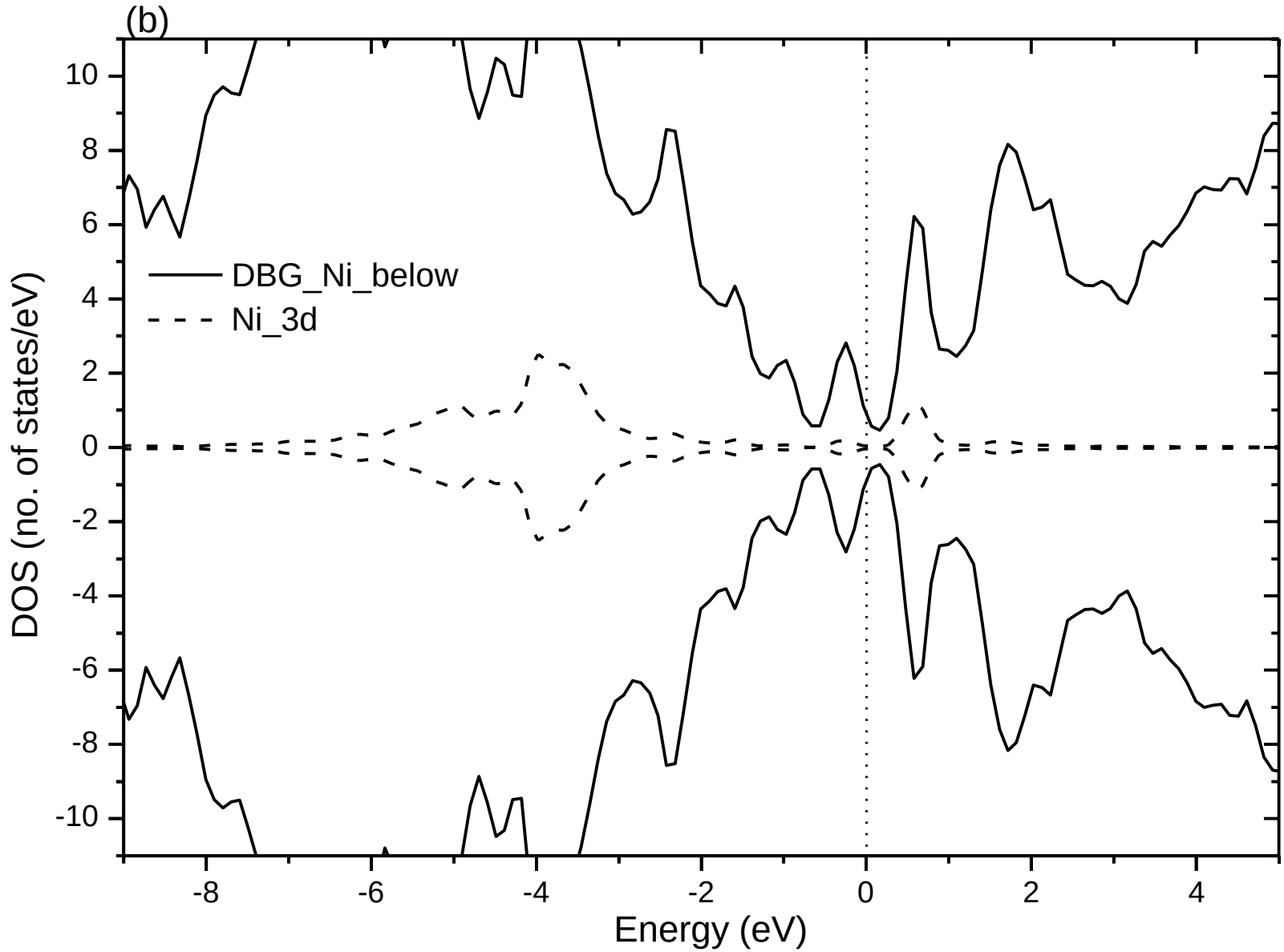
(b)
DBG_Ni_below
Ni_3d
DOS (no. of states/eV)
Energy (eV)
10
8
6
4
2
0
-2
-4
-6
-8
-10
-8
-6
-4
-2
0
2
4

Fig. S2(b)

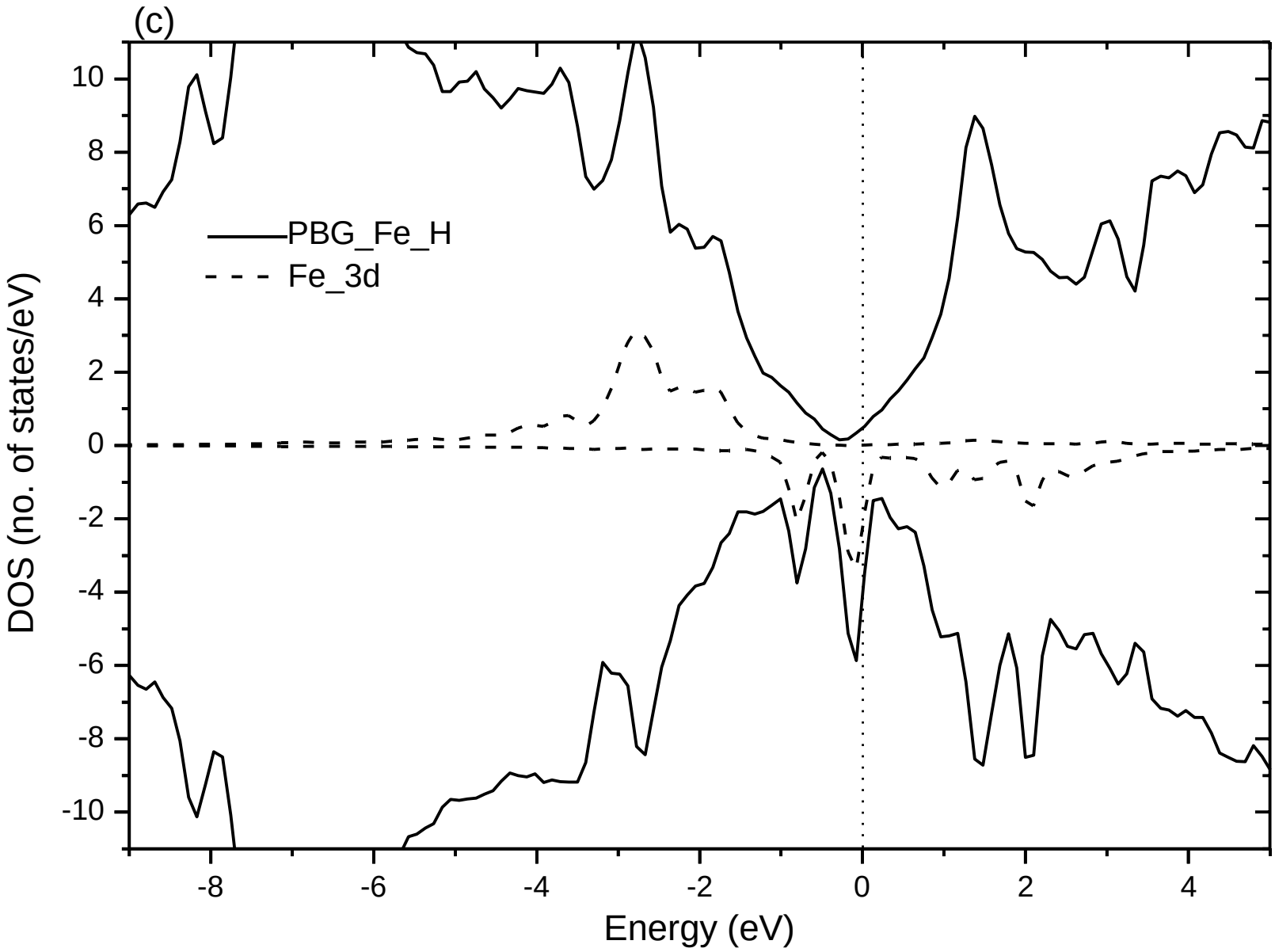
(c)
PBG_Fe_H
Fe_3d
DOS (no. of states/eV)
Energy (eV)
10
8
6
4
2
0
-2
-4
-6
-8
-10
-8
-6
-4
-2
0
2
4

Fig. S2(c)

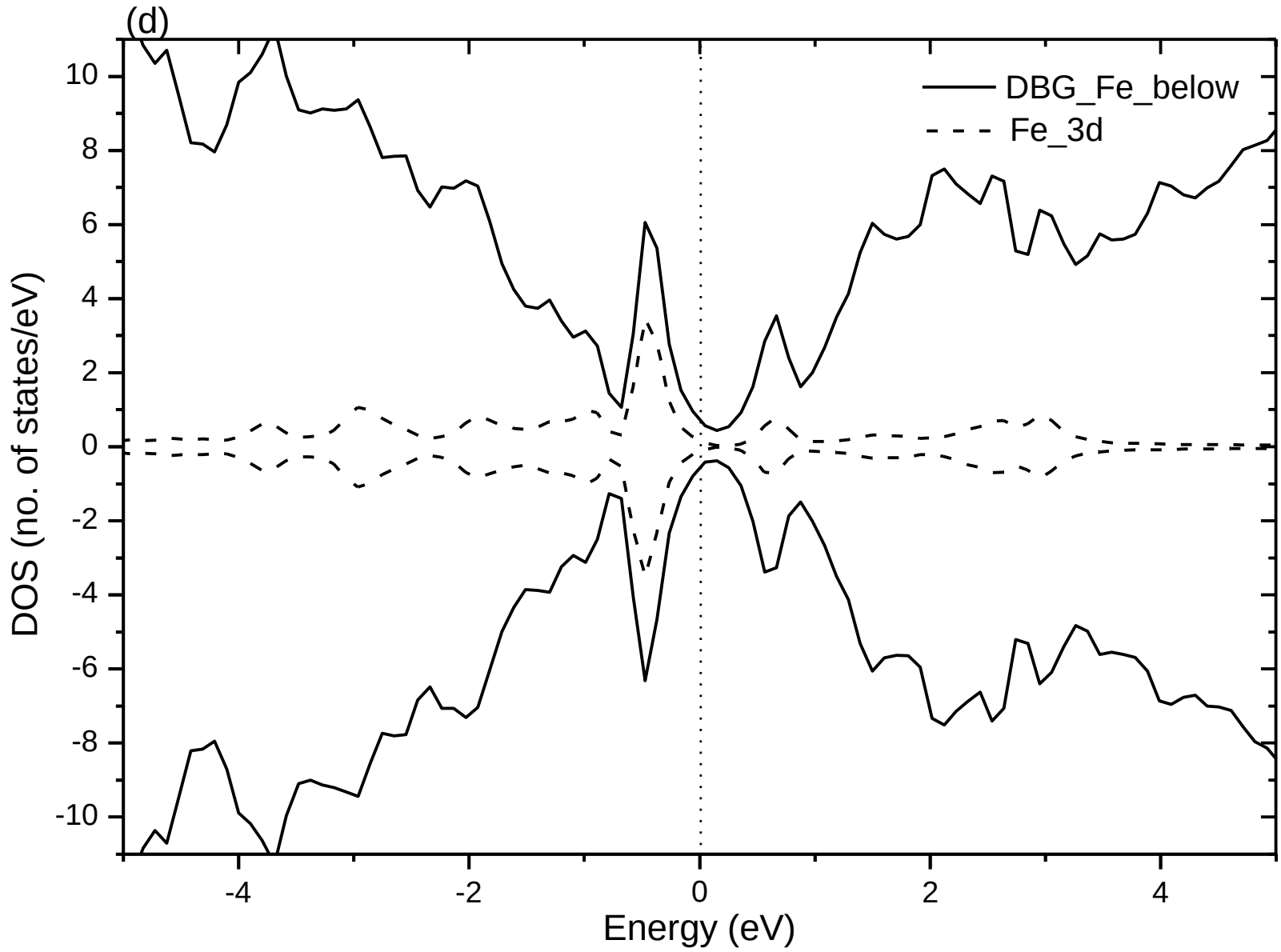
(d)
DBG_Fe_below
Fe_3d
DOS (no. of states/eV)
Energy (eV)
10
8
6
4
2
0
-2
-4
-6
-8
-10
-4
-2
0
2
4

Fig. S2(d)