

Fig. 1 Figure (a) is top and side view of NiI_2 structure. Figure (b) is standard electronic band structure and figure (c) is the projected band structure, where orange line is the d orbital of Ni and the green line is the p orbital of I. Figures (d) and (e) are the electronic band structure of NiI_2 with Hubbard correction, where $U=2$ and $J=0.8$ and $U=4$ and $J=0.8$, respectively.

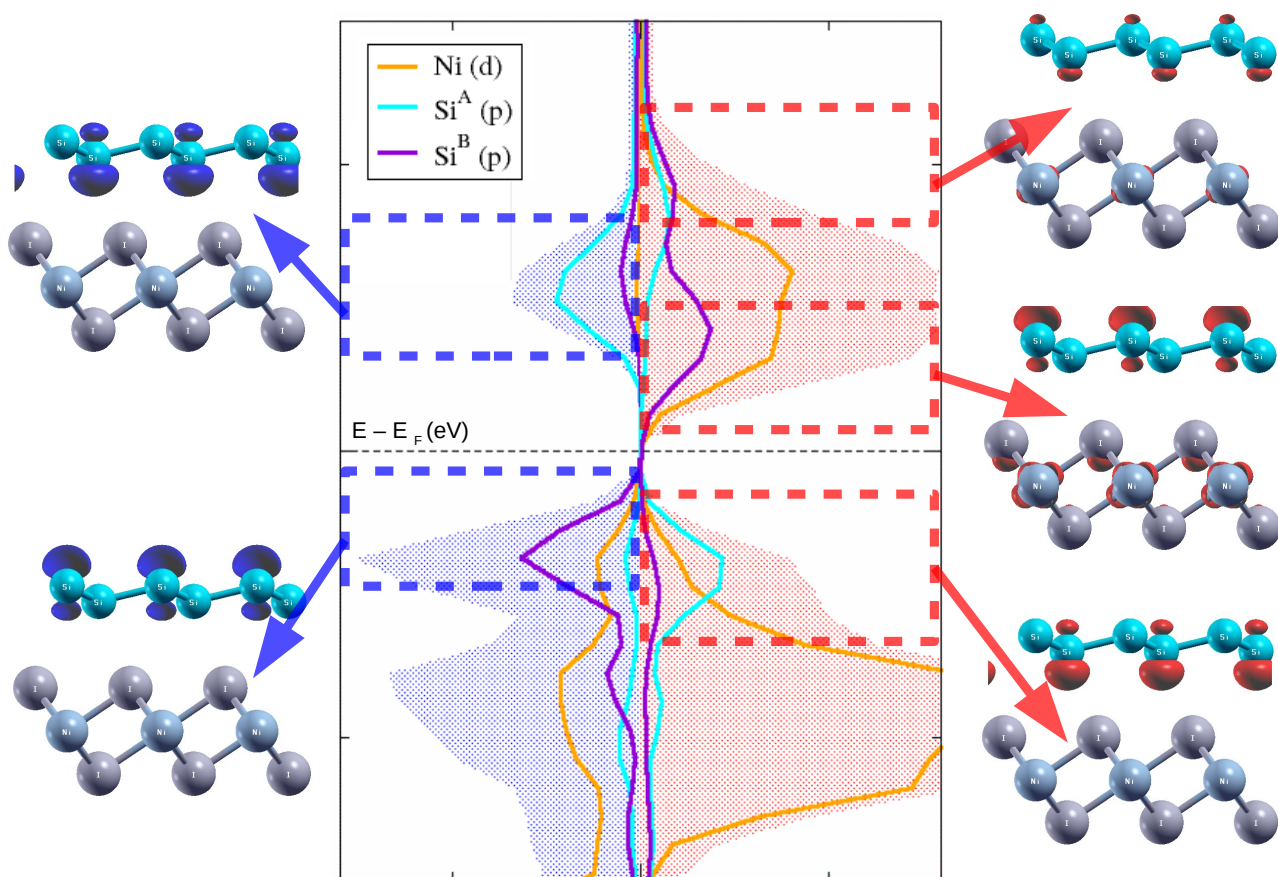


Fig. 2 PDOS of the vdW heterostructure. We also show the electronic charge density for the peak in the valence band and conduction band near to the Energy Fermi.

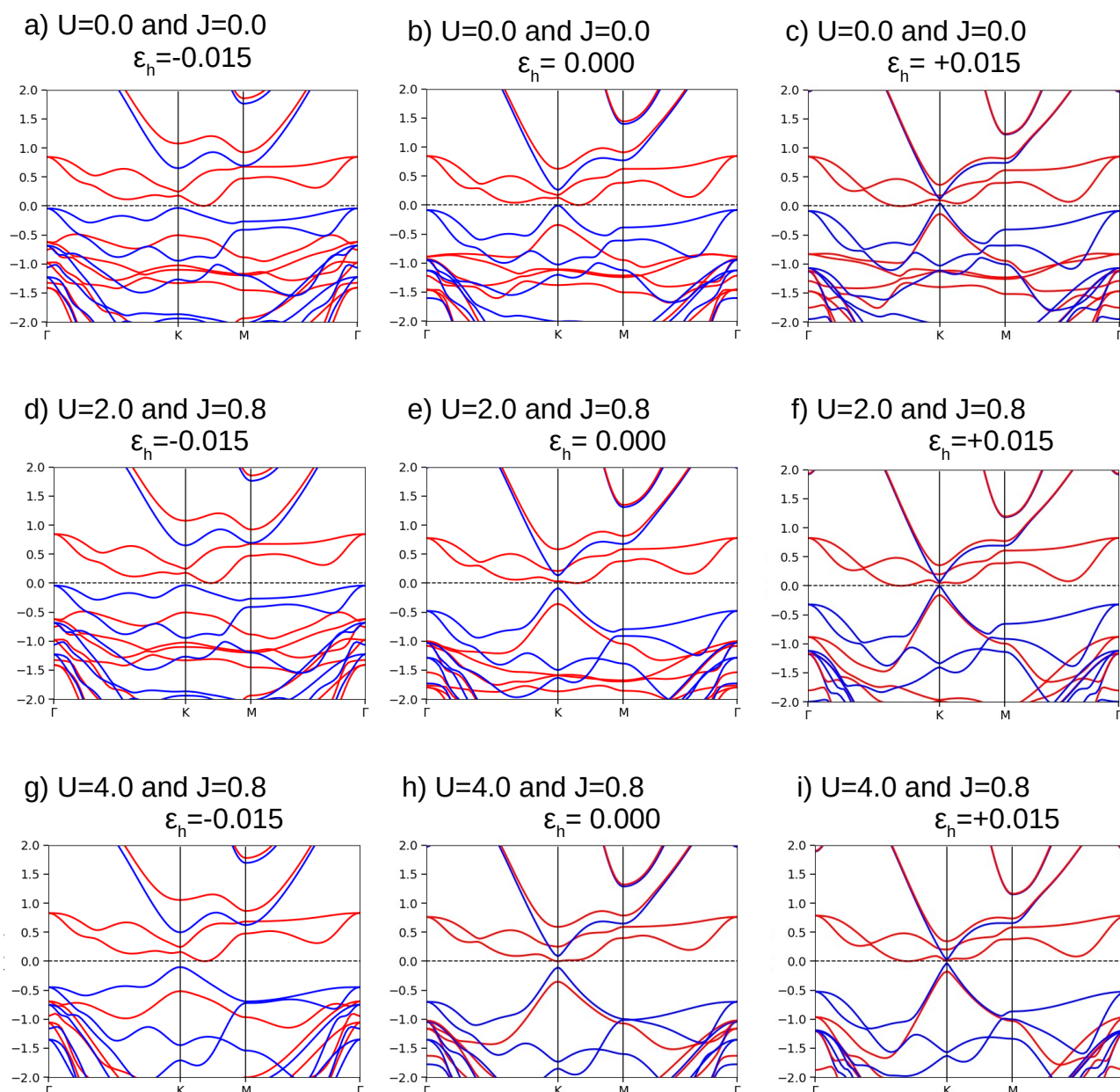


Fig. 3 Electronic band structure for the vdW heterostructures for different values of U and J under vertical strain.