

A – PDOS and PLDOS images

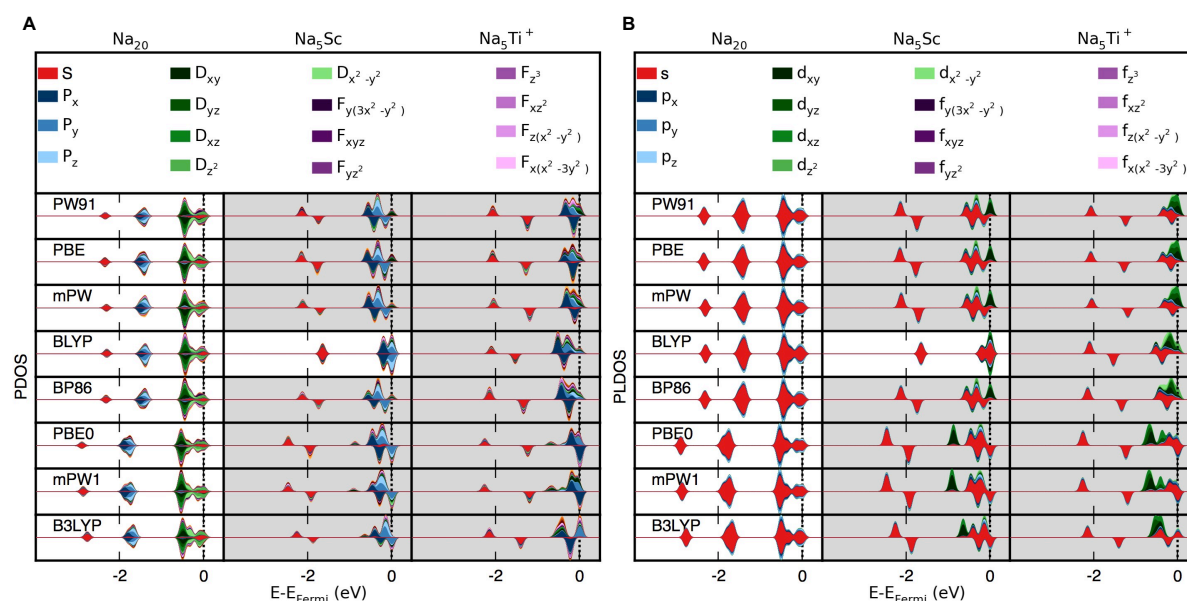


Figure 9: Angular momentum resolved density of states images for the Na_{20} , Na_5Sc and Na_5Ti^+ clusters for a host of exchange-correlation functionals. Subplot A presents the PDOS images where the projection is centred on the centre of mass of the cluster and subplot B presents the PLDOS images where the projections are centred on the atom centres themselves. The positive figures for each plot are the projection values for the spin-up Kohn-Sham states and the negative values are the projection values for the spin-down Kohn-Sham states. For all of the plots the a white plot face colour indicates that the lowest energy multiplicity is a singlet whereas a grey face colour is indicative of higher multiplicities.

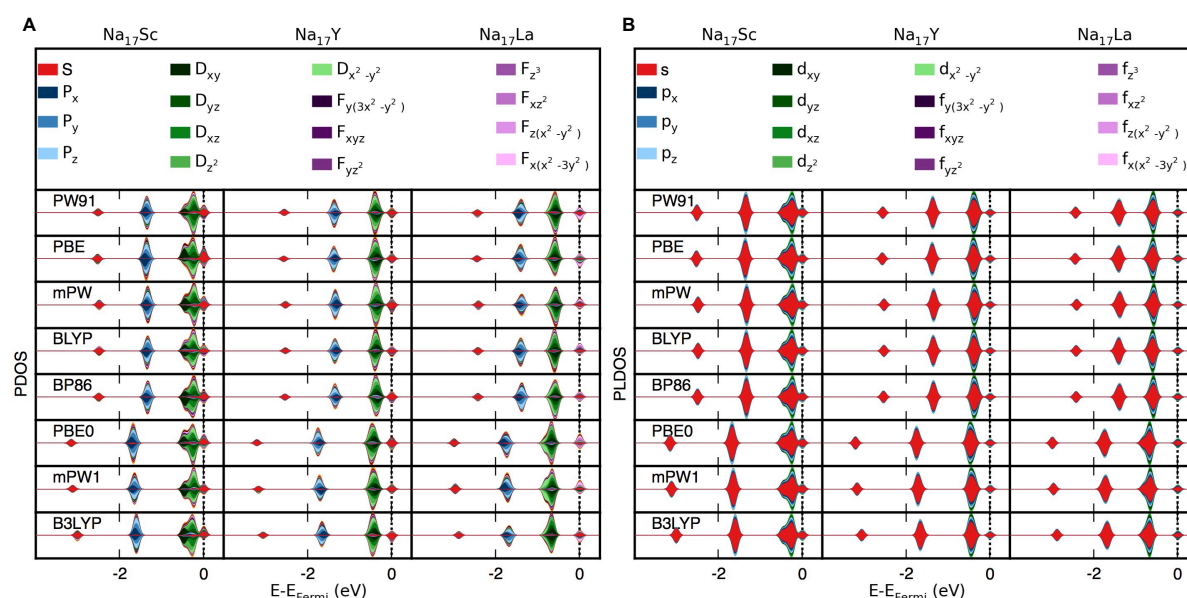


Figure 10: Angular momentum resolved density of states images for the Na_{17}Sc , Na_{17}Y and Na_{17}La clusters for a host of exchange-correlation functionals. Subplot A presents the PDOS images where the projection is centred on the centre of mass of the cluster and subplot B presents the PLDOS images where the projections are centred on the atom centres themselves. The positive figures for each plot are the projection values for the spin-up Kohn-Sham states and the negative values are the projection values for the spin-down Kohn-Sham states. For all of the plots the a white plot face colour indicates that the lowest energy multiplicity is a singlet whereas a grey face colour is indicative of higher multiplicities.

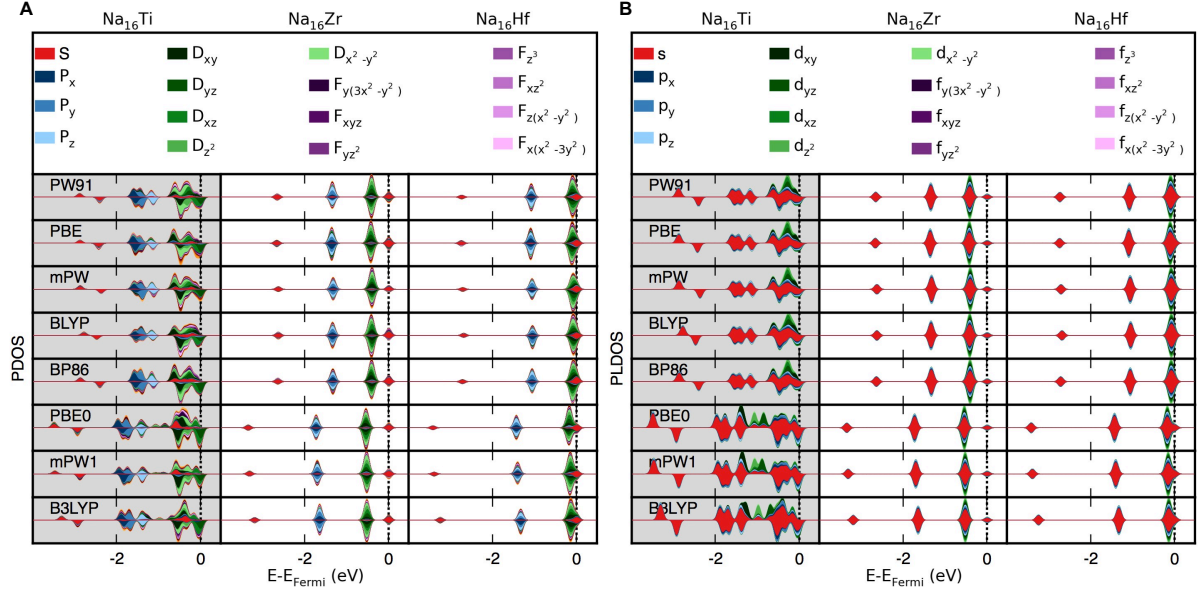


Figure 11: Angular momentum resolved density of states images for the Na_{16}Ti , Na_{16}Zr and Na_{16}Hf clusters for a host of exchange-correlation functionals. Subplot A presents the PDOS images where the projection is centred on the centre of mass of the cluster and subplot B presents the PLDOS images where the projections are centred on the atom centres themselves. The positive figures for each plot are the projection values for the spin-up Kohn-Sham states and the negative values are the projection values for the spin-down Kohn-Sham states. For all of the plots the a white plot face colour indicates that the lowest energy multiplicity is a singlet whereas a grey face colour is indicative of higher multiplicities.

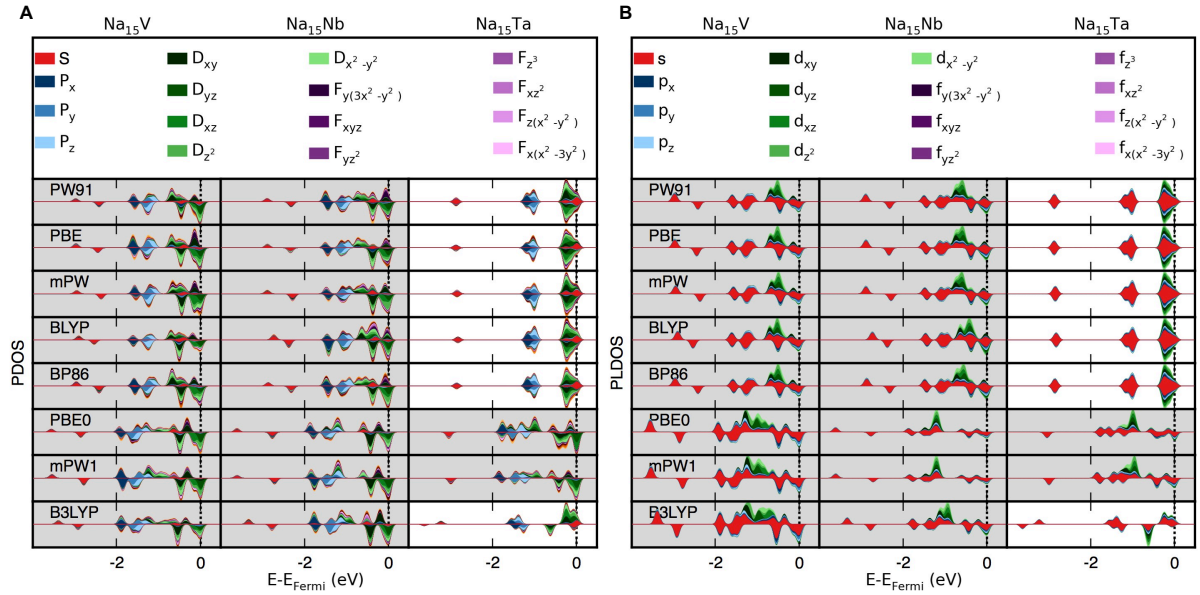


Figure 12: Angular momentum resolved density of states images for the Na_{17}Sc , Na_{17}Y and Na_{17}La clusters for a host of exchange-correlation functionals. Subplot A presents the PDOS images where the projection is centred on the centre of mass of the cluster and subplot B presents the PLDOS images where the projections are centred on the atom centres themselves. The positive figures for each plot are the projection values for the spin-up Kohn-Sham states and the negative values are the projection values for the spin-down Kohn-Sham states. For all of the plots the a white plot face colour indicates that the lowest energy multiplicity is a singlet whereas a grey face colour is indicative of higher multiplicities.

B – Projection Methodology

This section has the integrals which were used to obtain the weighting factors for the PDOS and PLDOS images. These integrals were solved numerically using self-written Monte-Carlo code.

Projected Density of States:

$$w_m^l = \left| \int_0^R \int_0^\pi \int_0^{2\pi} Y_m^l(\theta, \varphi) \psi(r, \theta, \varphi) r^2 \sin \theta \, d\theta d\varphi dr \right|^2$$

Projected Local Density of States:

$$w_m^l = \sum_N \left| \int_0^{R_N} \int_0^\pi \int_0^{2\pi} Y_m^l(\theta, \varphi) \psi(r_N, \theta, \varphi) r_N^2 \sin \theta \, d\theta d\varphi dr_N \right|^2$$