

Fig. S1. Nine constructed lithiated $XY-M_2CO_2Li_2$ configurations

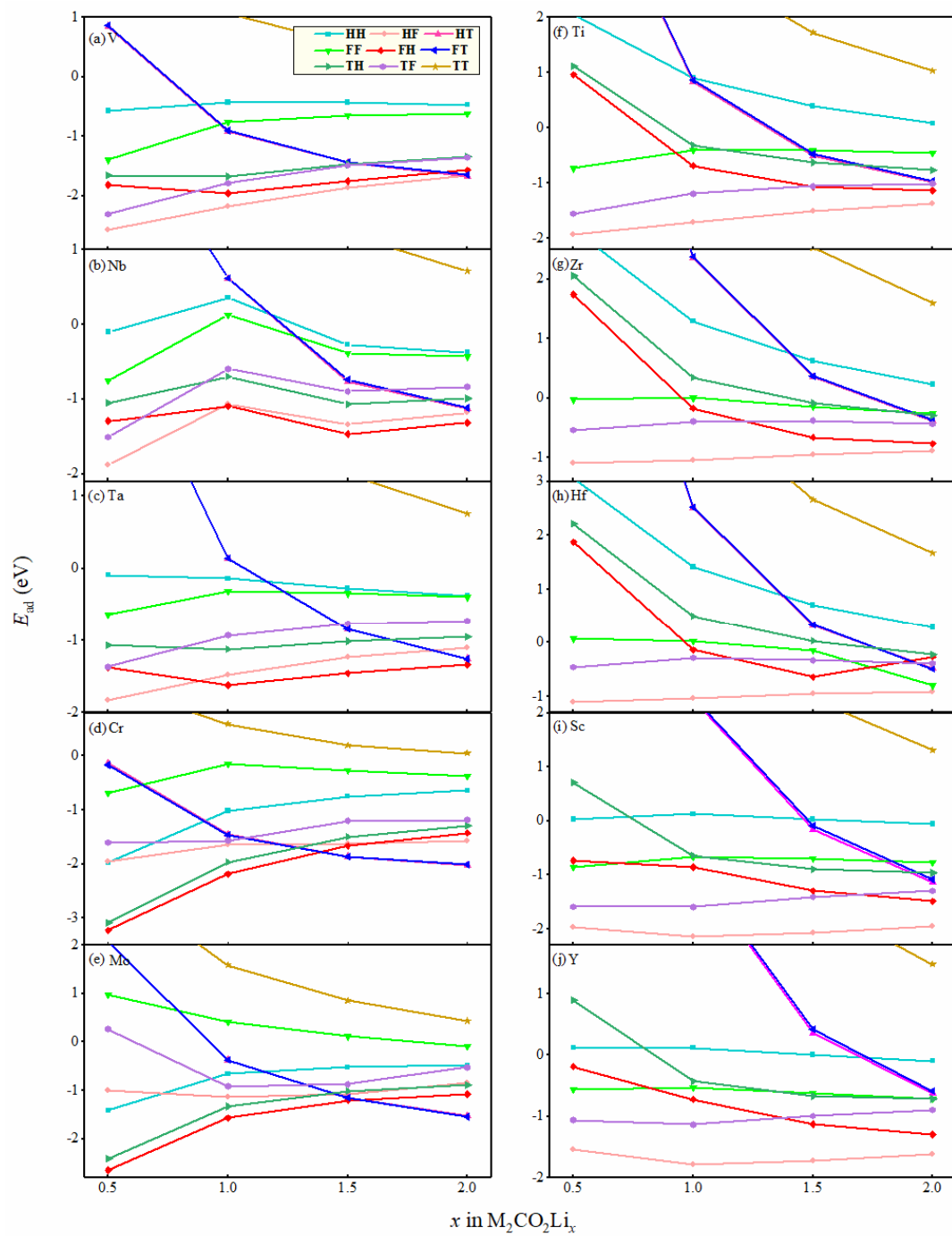
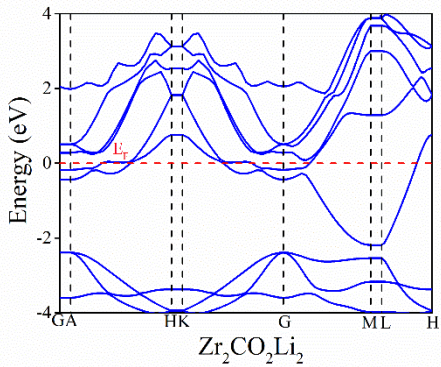
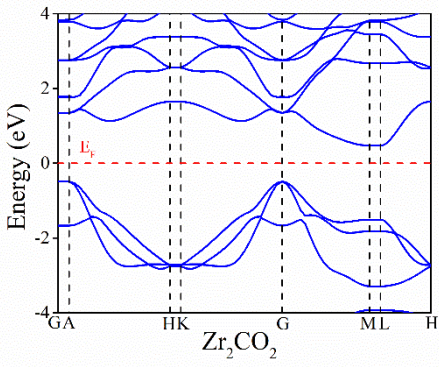
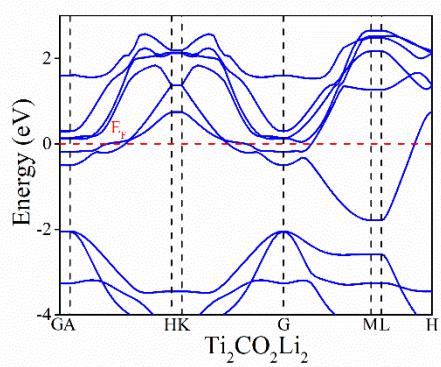
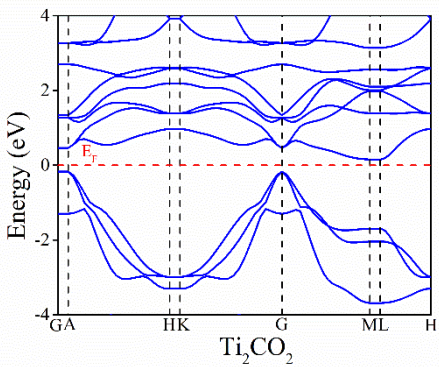
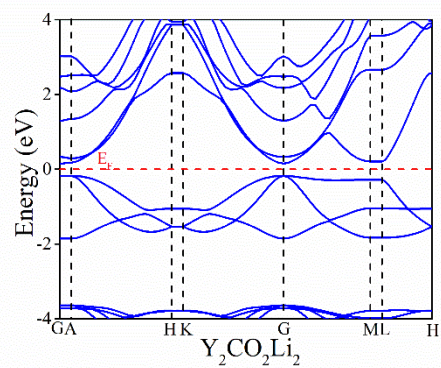
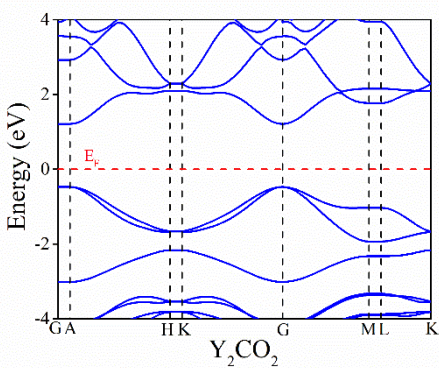
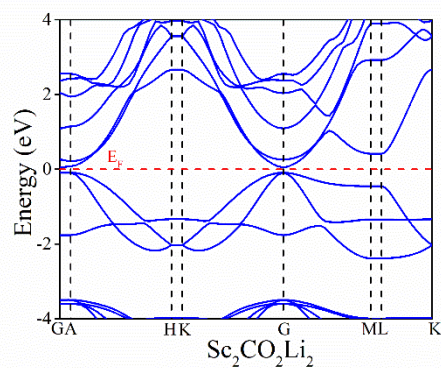
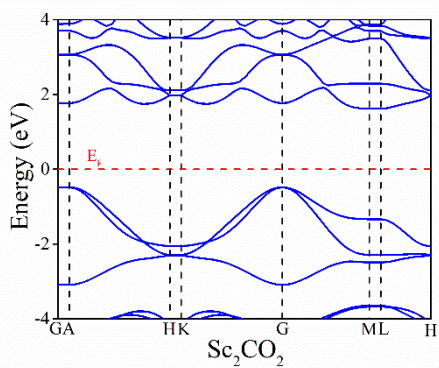
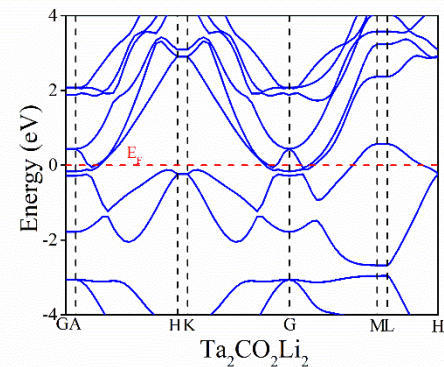
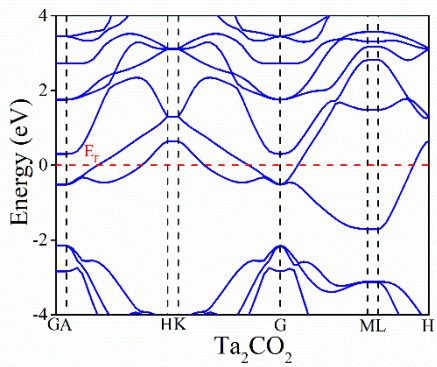
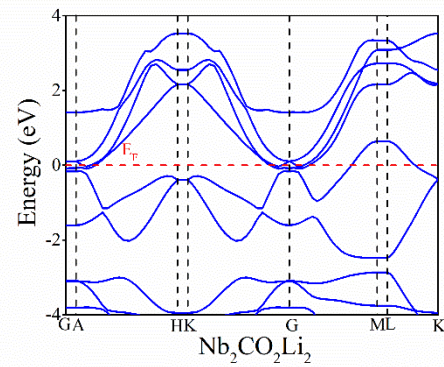
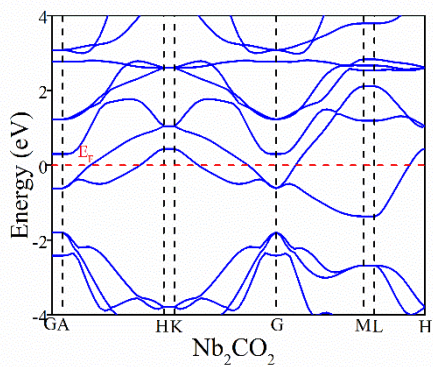
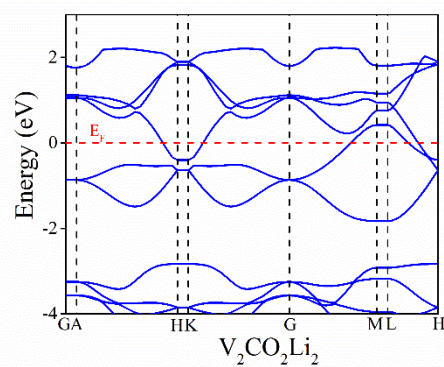
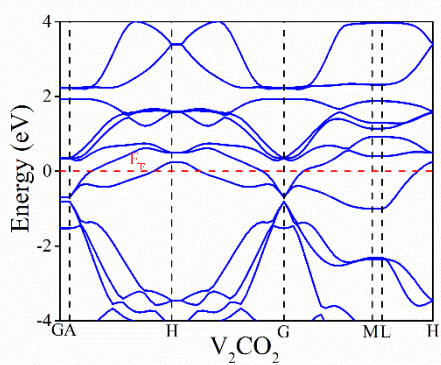
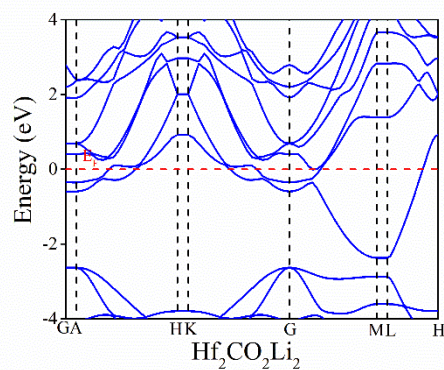
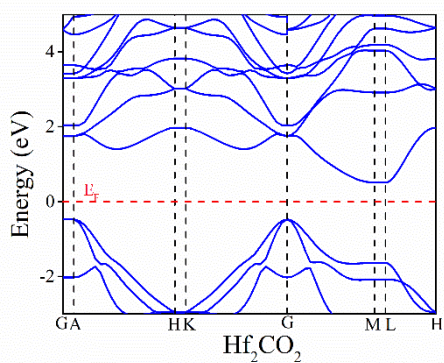


Fig. S2. Adsorption energies of different $M_2CO_2Li_x$ configurations with a variable of Li contents (x values)





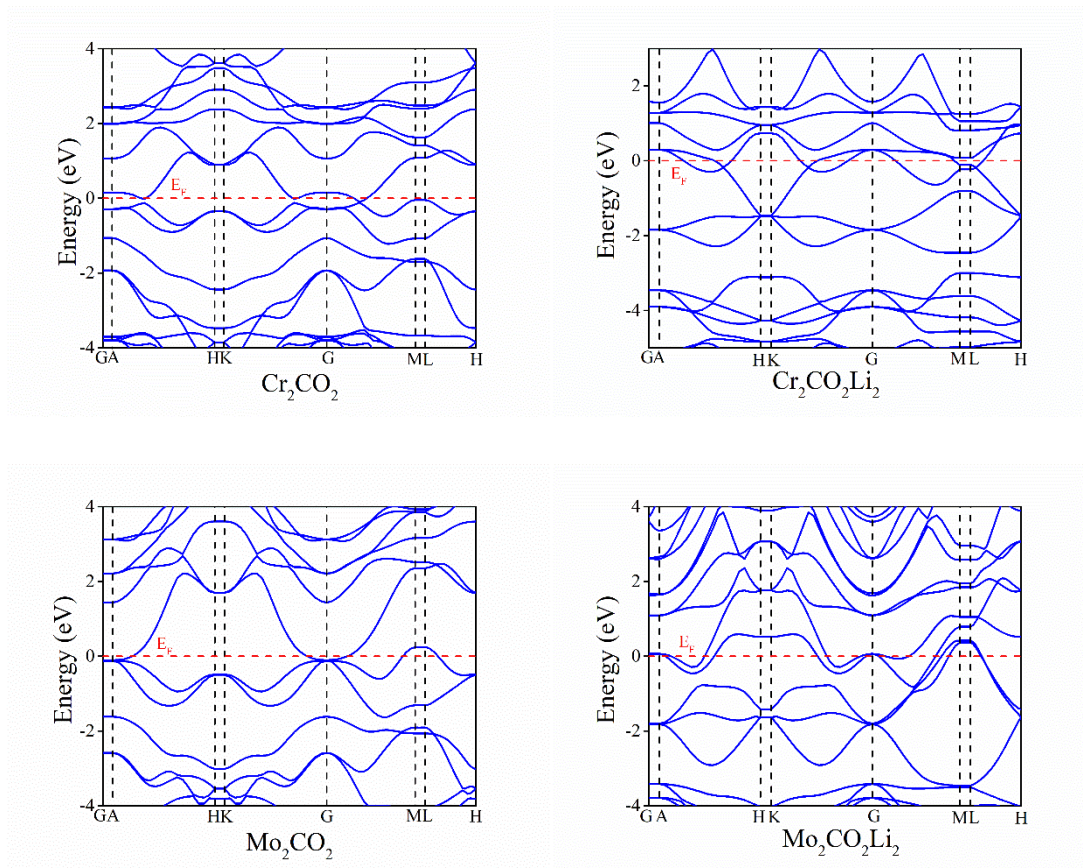


Fig. S3. Band structures of different MXenes before and after lithiation.