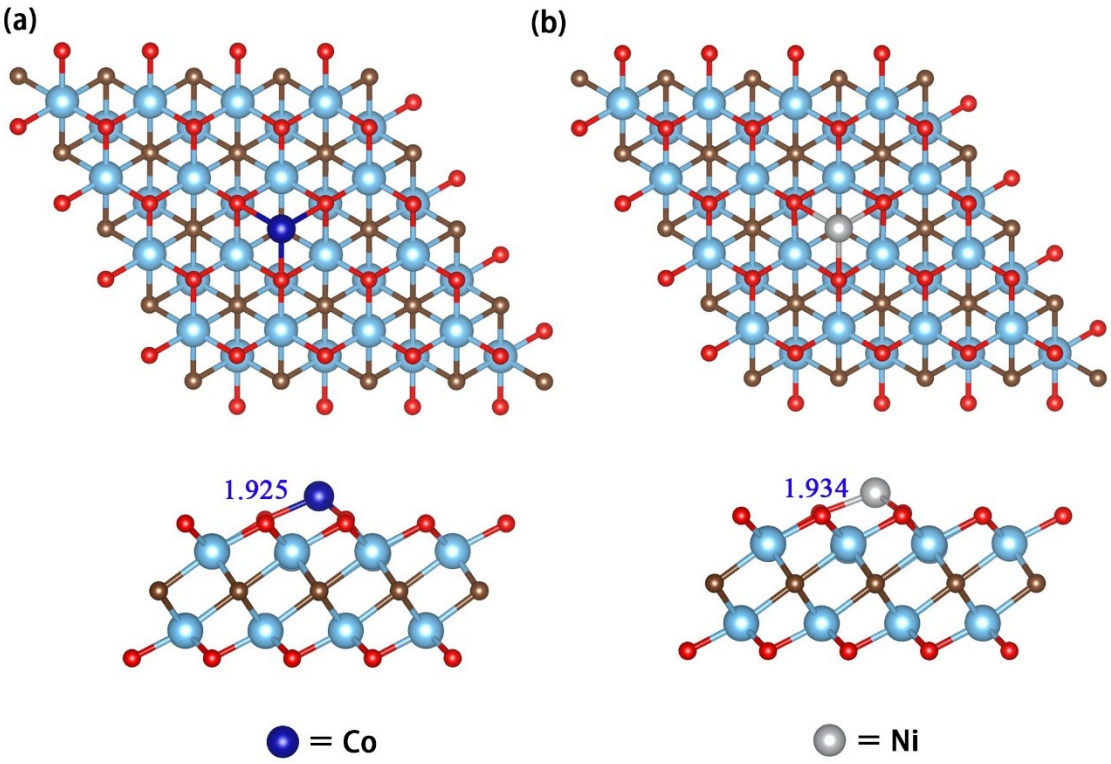

Figure S1. The most stable adsorption configuration of Co(a) and Ni(b) atoms on Ti_2CO_2.

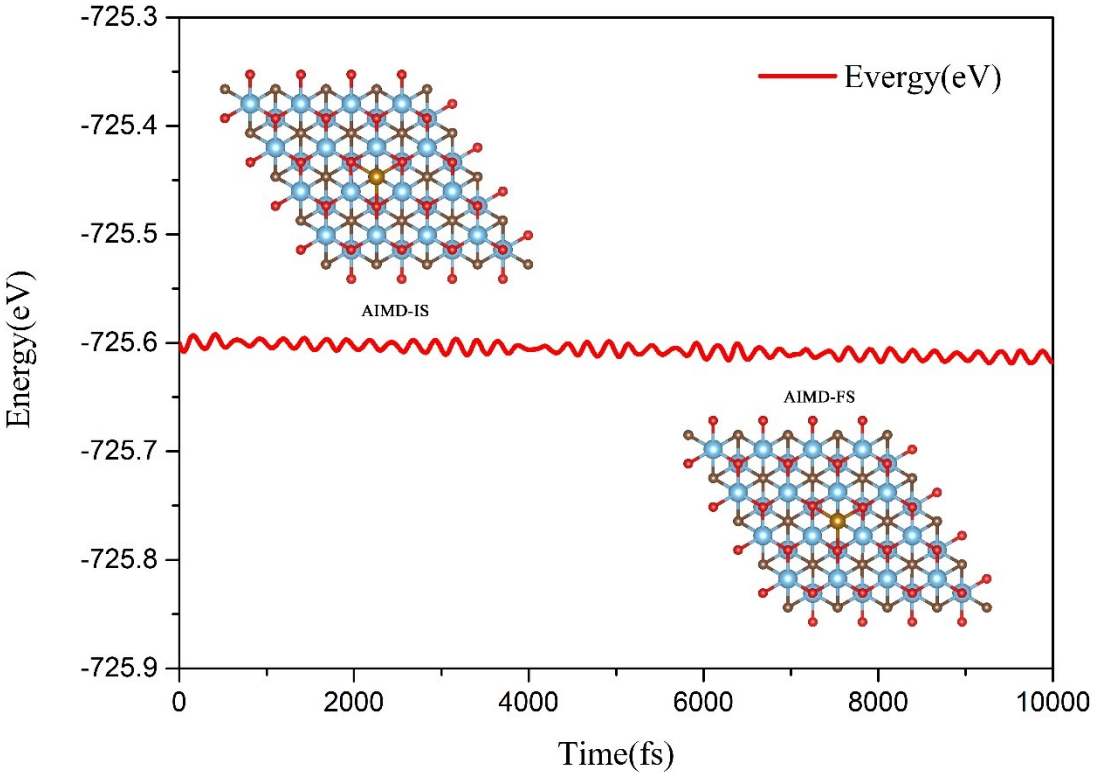

Figure S2. Energy curve within 10 ps at 300 K by AIMD(Ab initio molecular dynamics), the initial state(IS), and final state(FS) are shown in the figure.

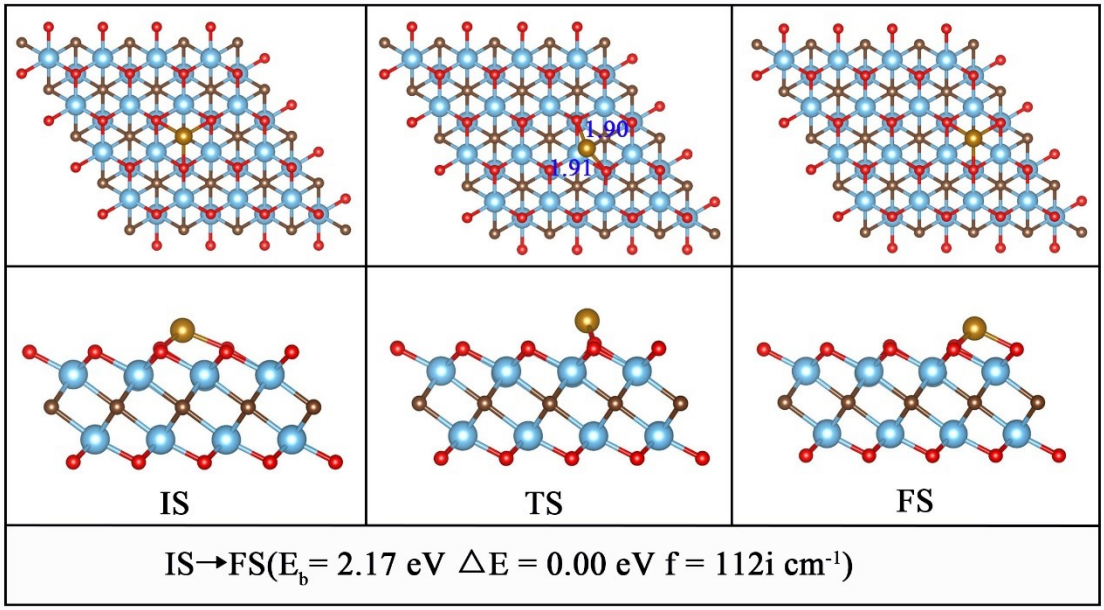

Figure S3. The schematic energy distribution of a single Fe atom moving from the most stable position(Site-B) on the Fe_1/Ti_2CO_2 monolayer to its adjacent position(Site-B).