Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information (SI)

Substitutional transition metal doping in $MoSi_2N_4$ monolayer: Structural, Electronic and Magnetic Properties

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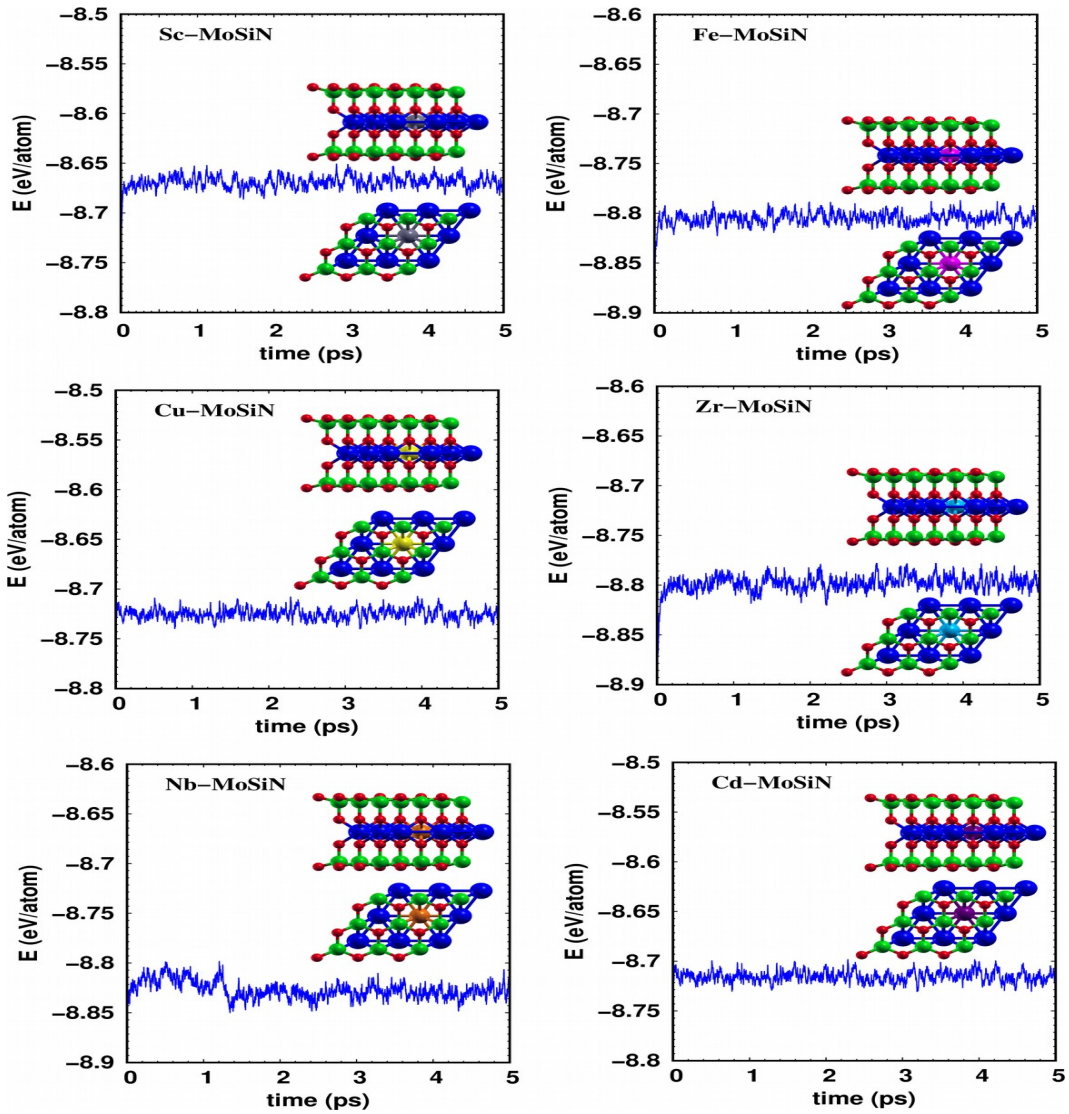

Figure S1. Ab-initio molecular dynamics at 300 K for the Sc-MoSiN, Fe-MoSiN, Cu-MoSiN, Zr-MoSiN, Nb-MoSiN, Cd-MoSiN. The side and top views of atomic structures after AIMD simulation are the inset figures in the corresponding structures (N (red), Si (green), Mo (blue) and TM dopant (Sc (grey), Fe (pink), Cu (yellow), Zr (sky-blue), Nb (dark-yellow) and Cd (violet)).

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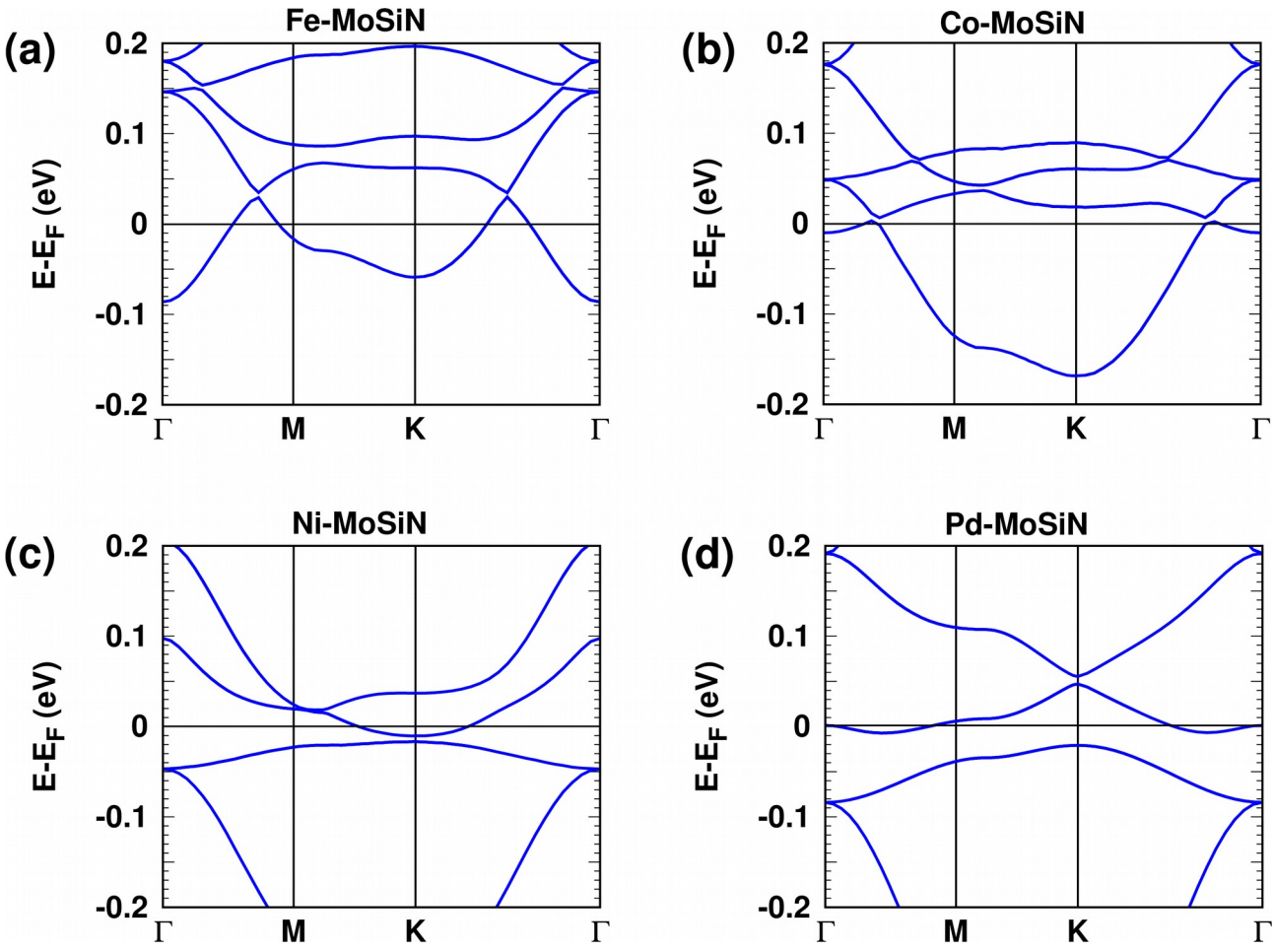

Fig. S2 The band structure of (a) Fe-, (b) Co-, (c) Ni- and (d) Pd-MoSiN monolayers with spin-orbit coupling effect.

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