Supporting Information

Adsorption of methylisocyanate and ethylisocyanate on Co-decorated TiS_2 monolayer: Understanding chemical interactions using DFT and COHP

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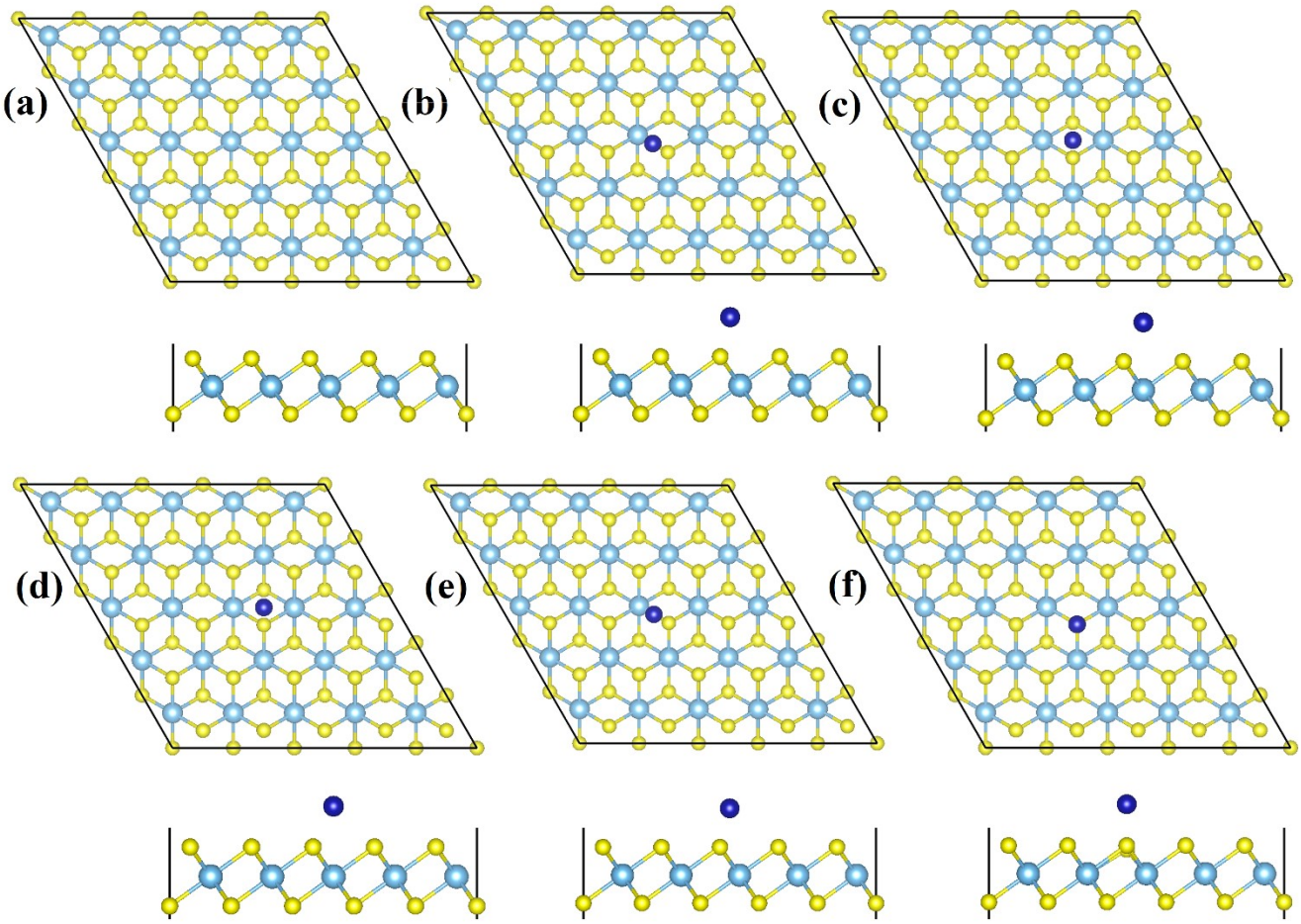

Figure S1: Top and side views of initial structures of (a) pristine-TiS_2 and different configurations of Co-decorated TiS_2, (b) bridge site, (c) hollow site, (d) lower S site, (e) Ti top site, (f) upper S site

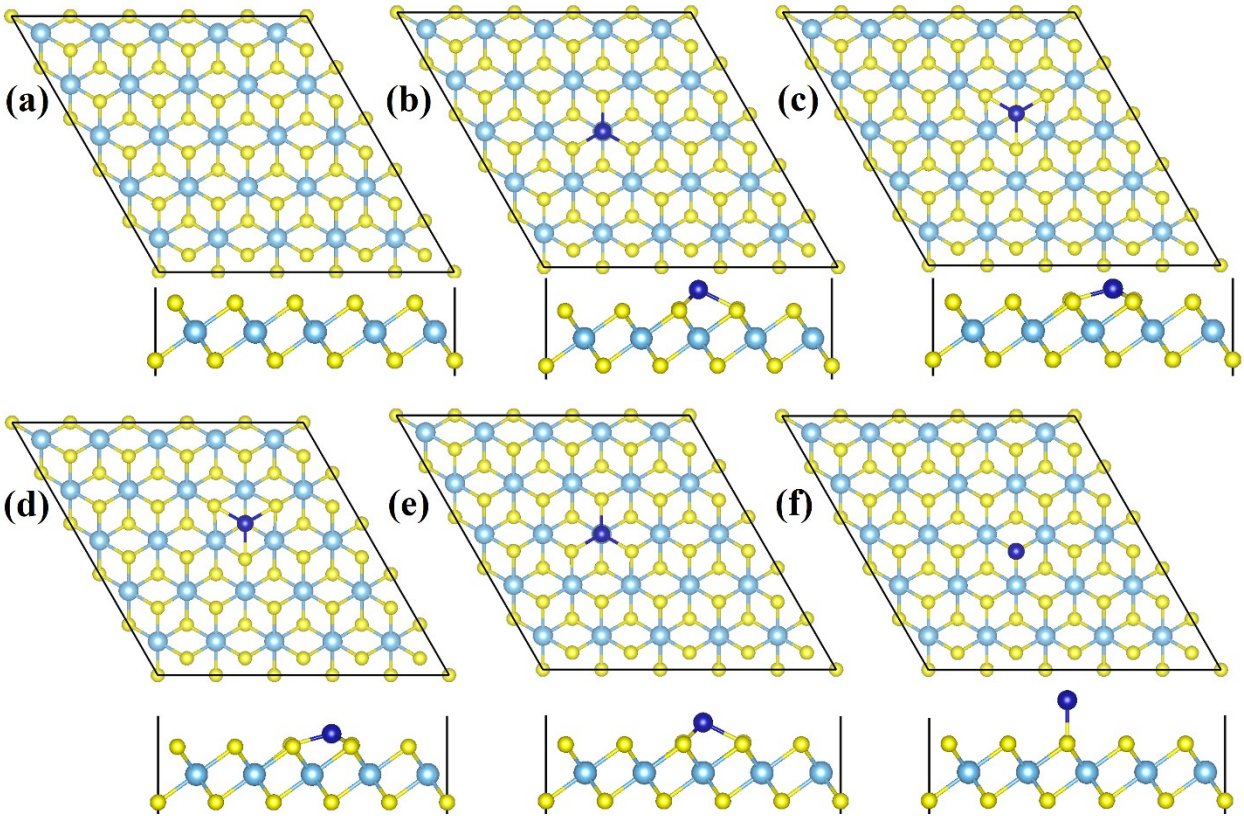

Figure S2: Top and side views of relaxed structures of (a) pristine-TiS_2 and different configurations of Co-decorated TiS_2, (b) bridge site, (c) hollow site, (d) lower S site, (e) Ti top site, (f) upper S site

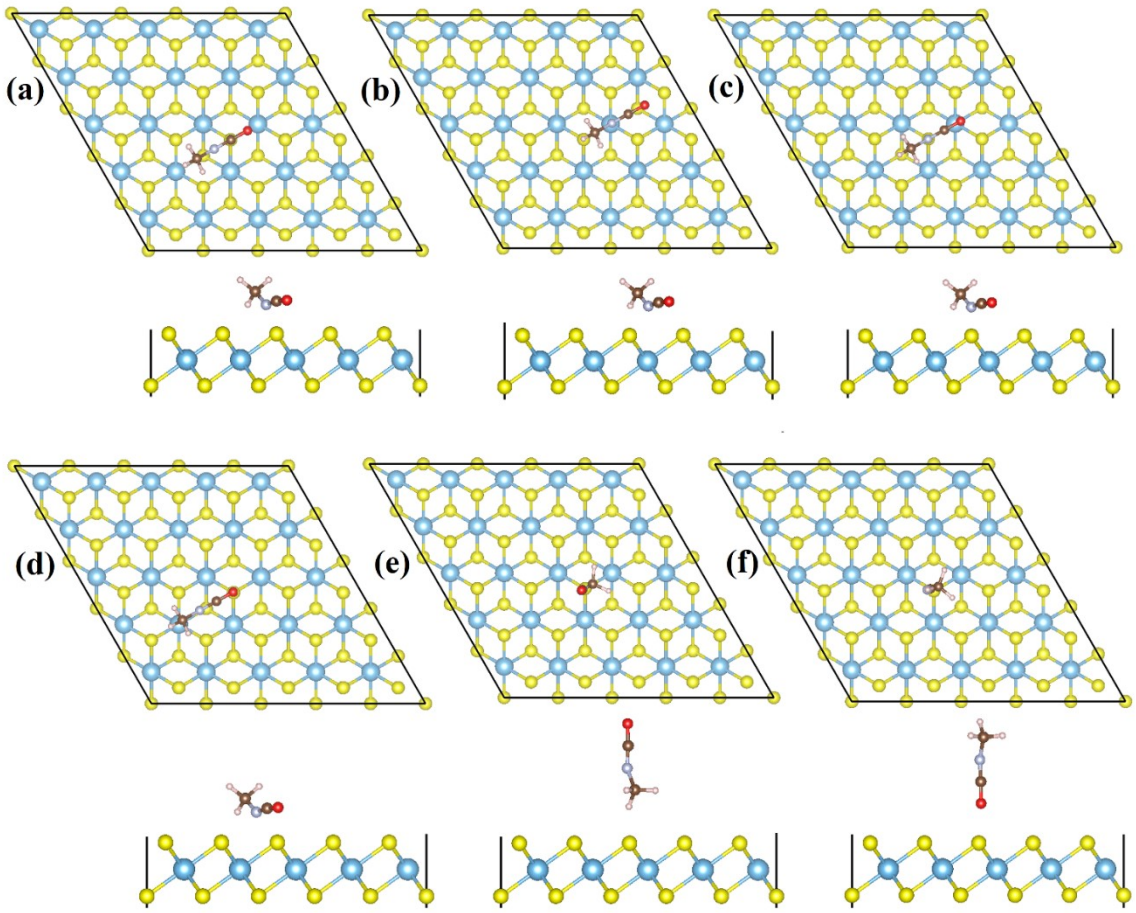

Figure S3: Top and side views of the initial adsorption configurations of methyl isocyanate (C_2H_3NO) on the pristine-TiS_2 (p-TiS_2) surface. Horizontal (h) configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular (v) configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface

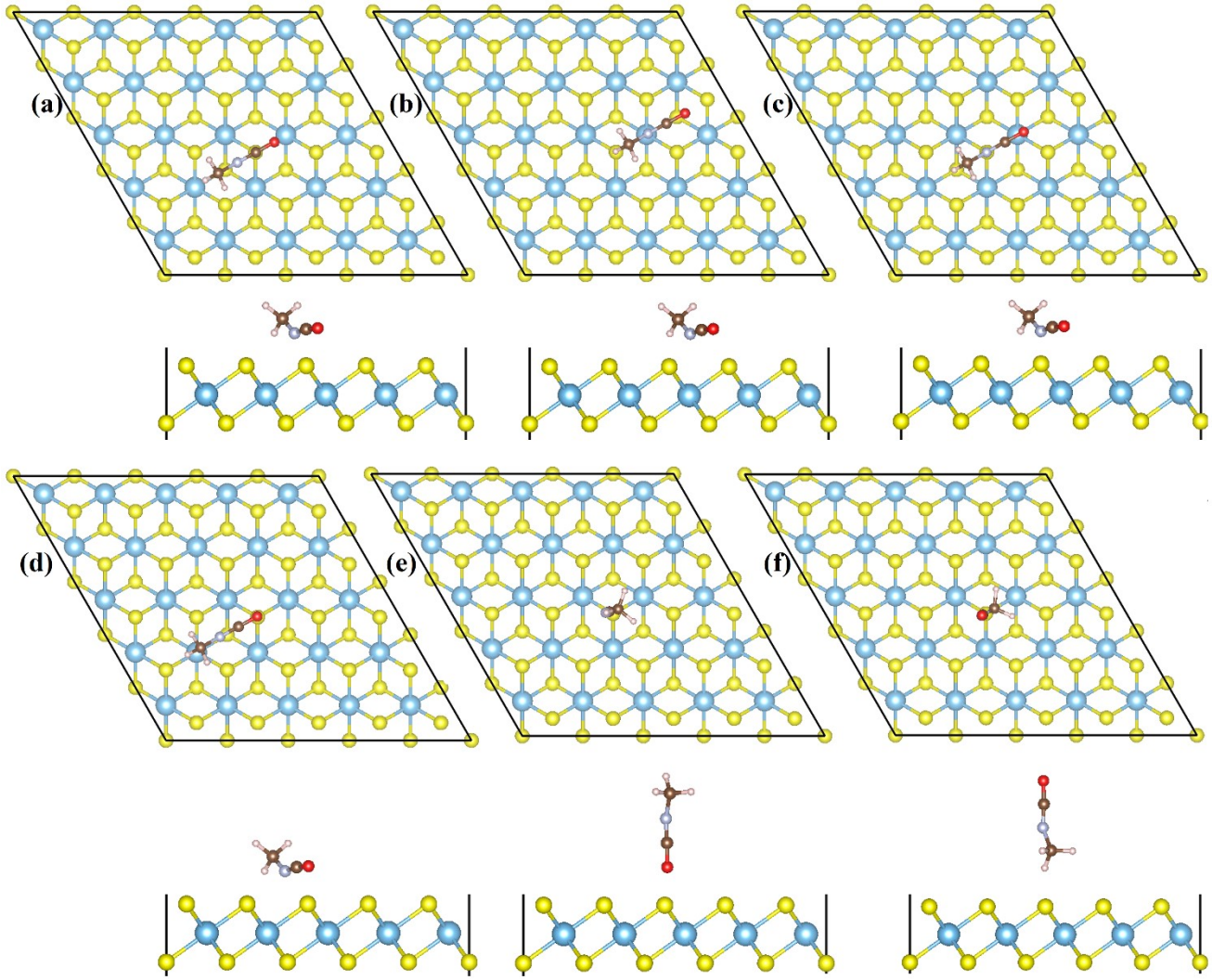

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Figure S4: Top and side views of the final adsorption configurations of methyl isocyanate (C_2H_3NO) on the pristine-TiS_2 (p-TiS_2) surface. Horizontal (h) configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular (v) configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface

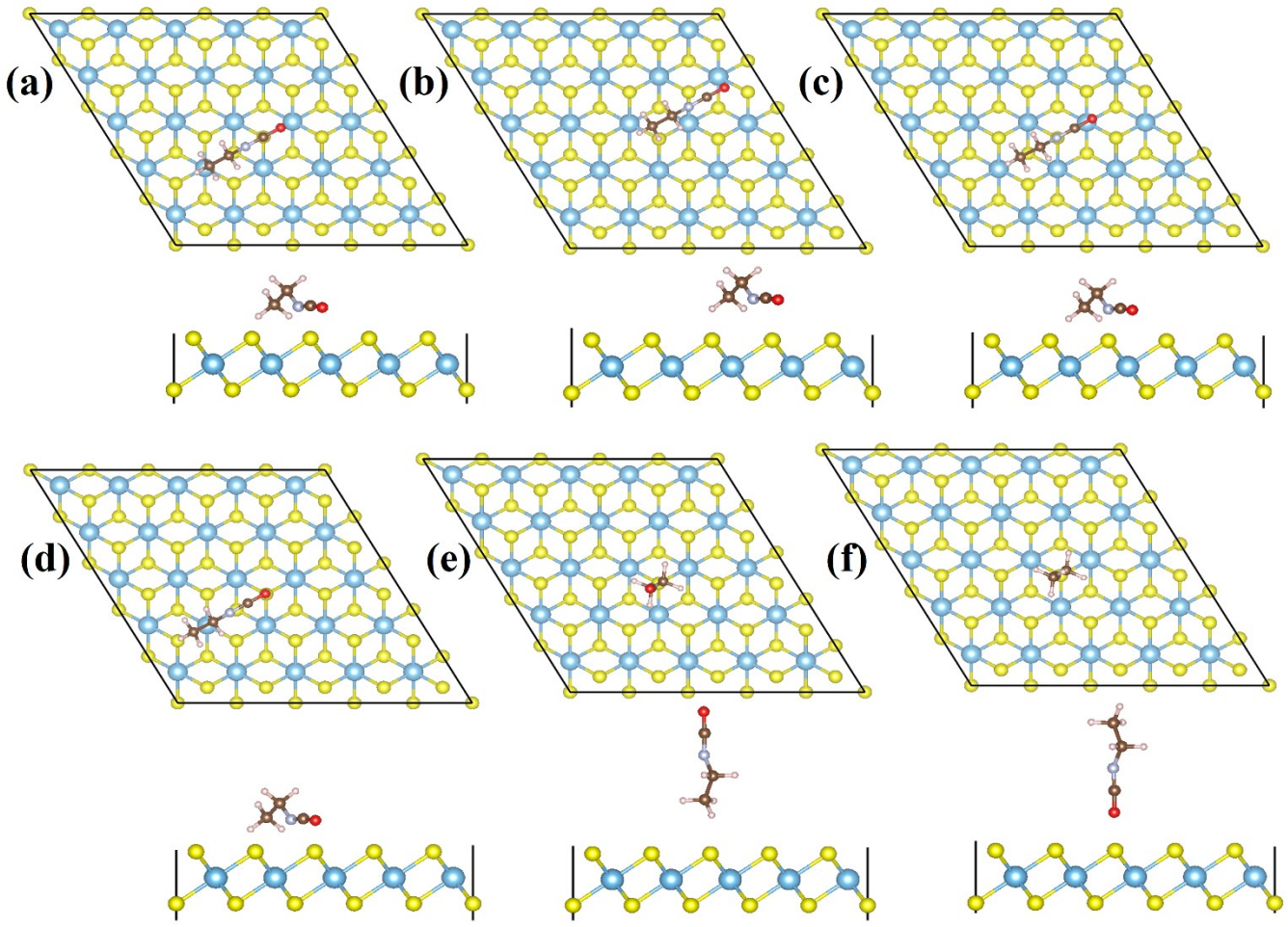

Figure S5: Top and side views of the initial adsorption configurations of ethyl isocyanate (C_3H_5NO) on the pristine-TiS_2 (p-TiS_2) surface. Horizontal (h) configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular (v) configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface

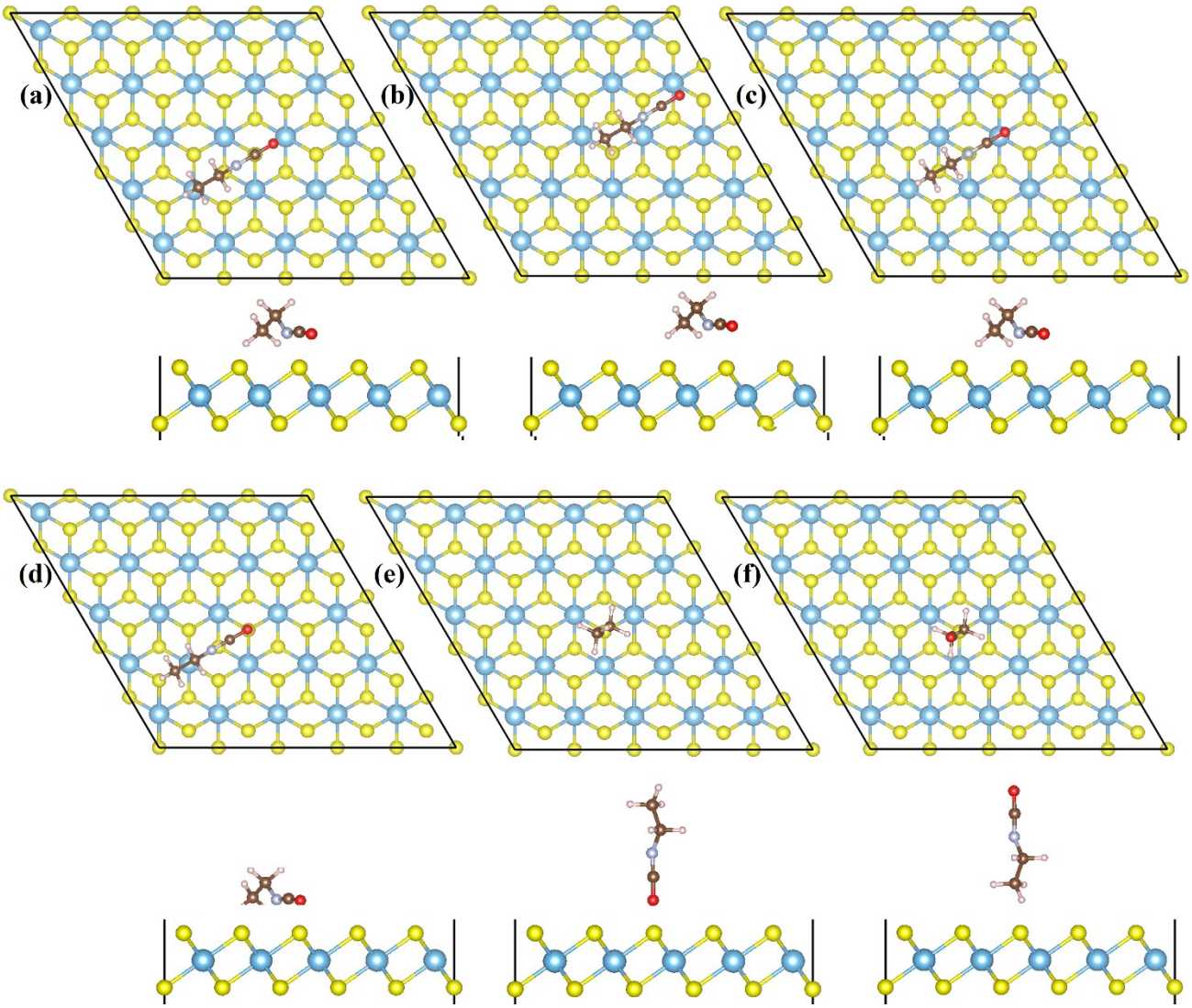

Figure S6: Top and side views of the initial adsorption configurations of ethyl isocyanate (C_3H_5NO) on the pristine-TiS_2 (p-TiS_2) surface. Horizontal (h) configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular (v) configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface

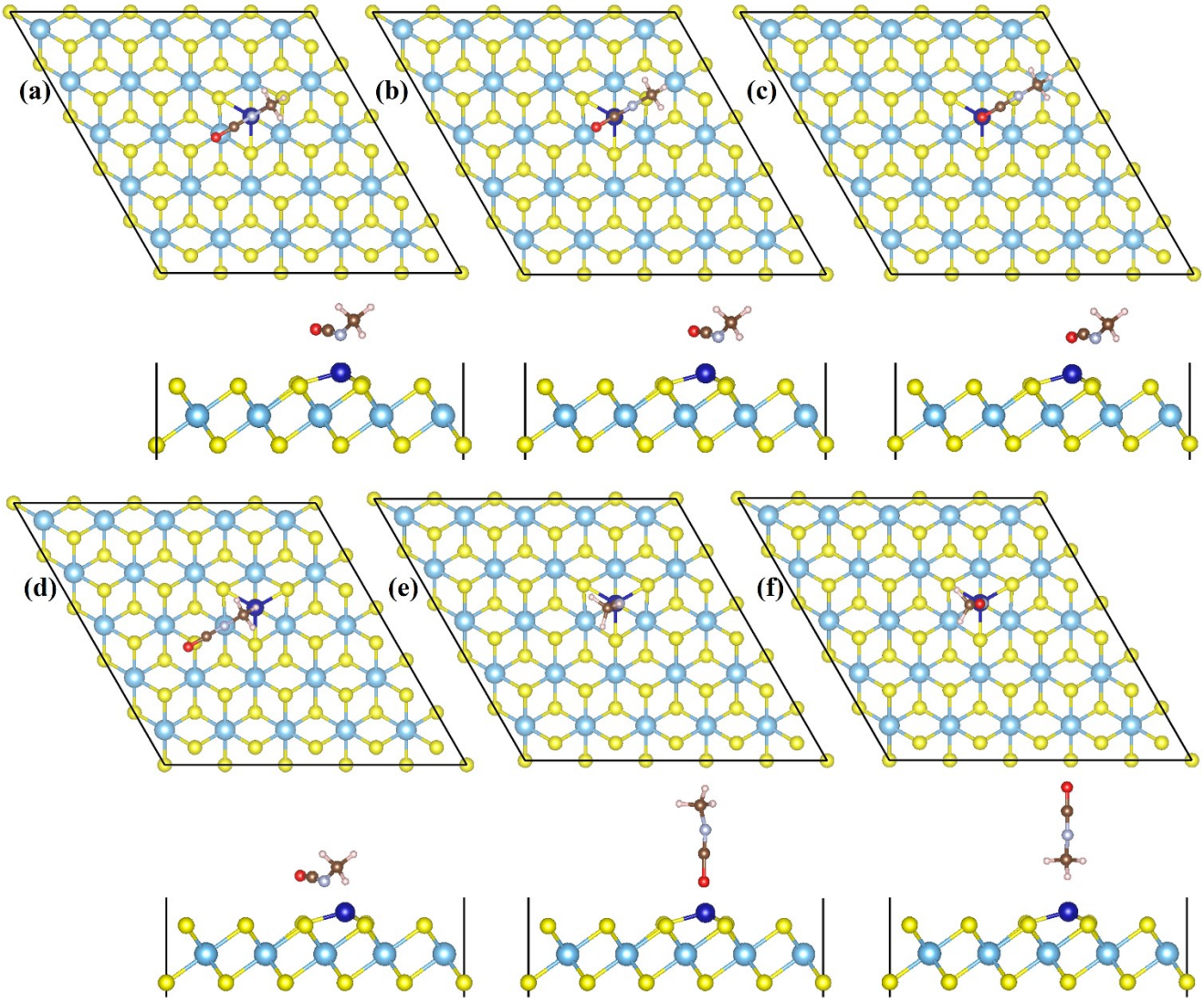

Figure S7: Top and side views of the initial adsorption configurations of methyl isocyanate (C_2H_3NO) on the Co-decorated-TiS_2 (Co-TiS_2) surface. Horizontal configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface.

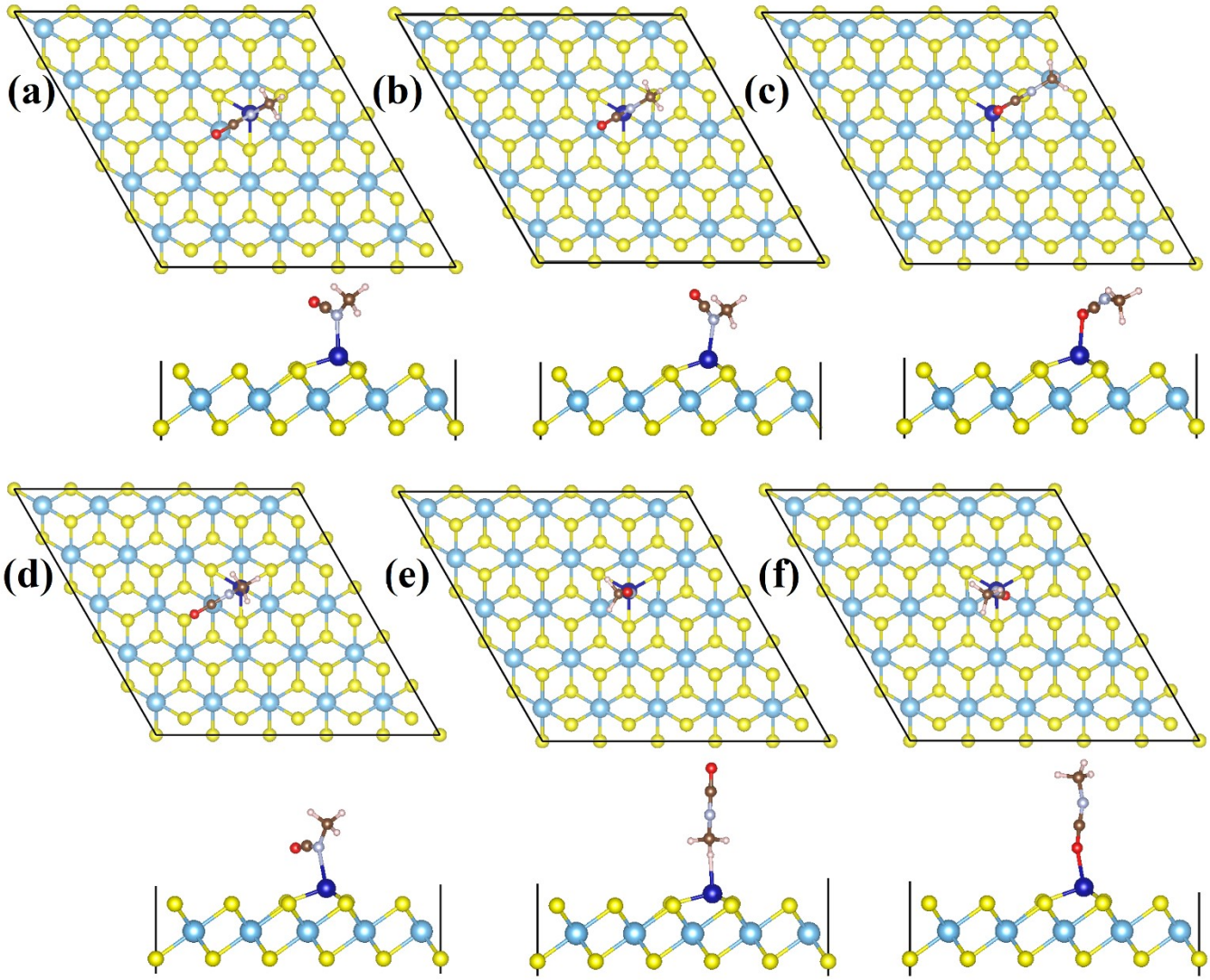

Figure S8: Top and side views of the final adsorption configurations of methyl isocyanate (C_2H_3NO) on the Co-decorated-TiS_2 (Co-TiS_2) surface. Horizontal configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface.

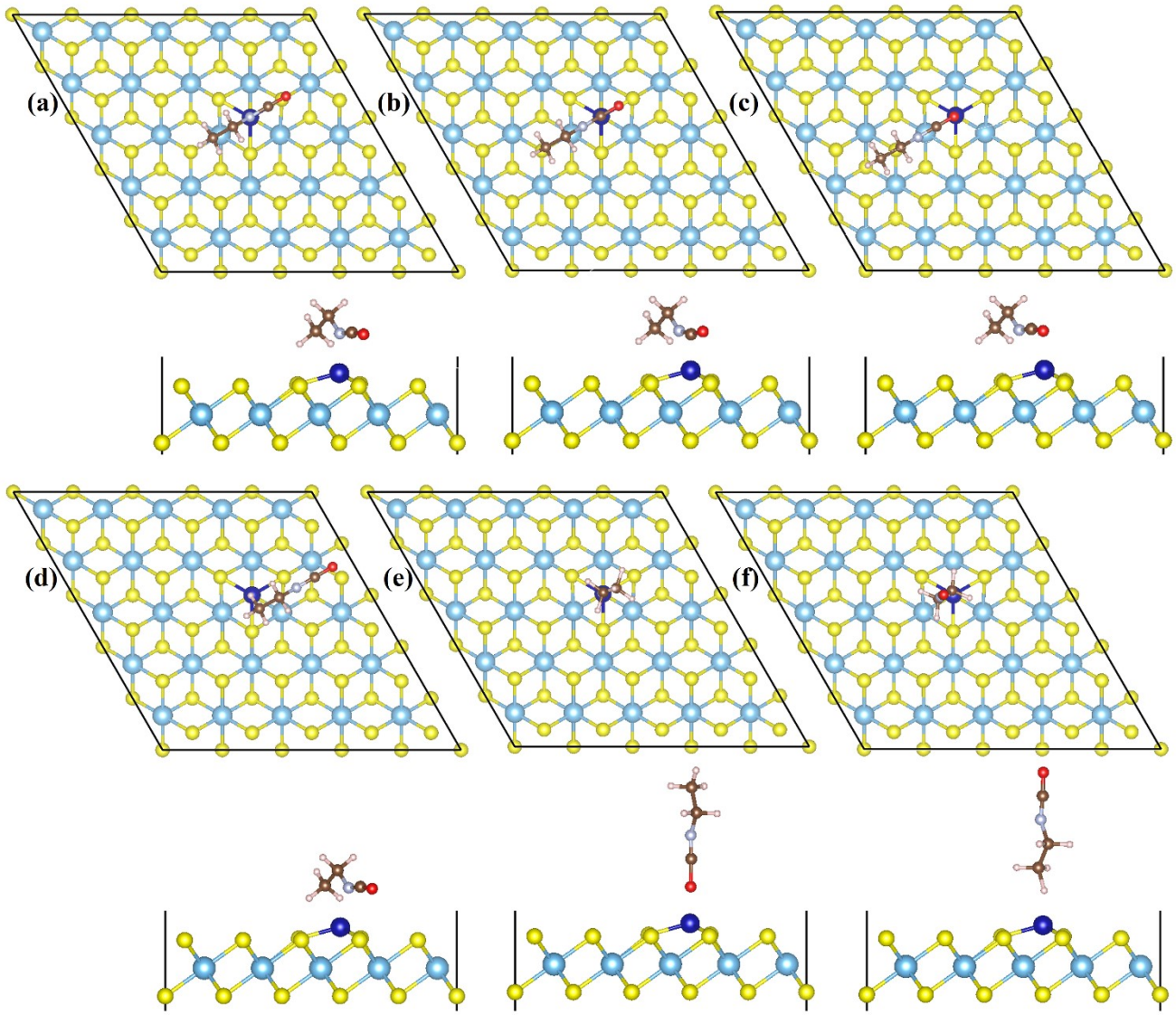

Figure S9: Top and side views of the initial adsorption configurations of ethyl isocyanate (C_3H_5NO) on the Co-decorated-TiS_2 (Co-TiS_2) surface. Horizontal configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface.

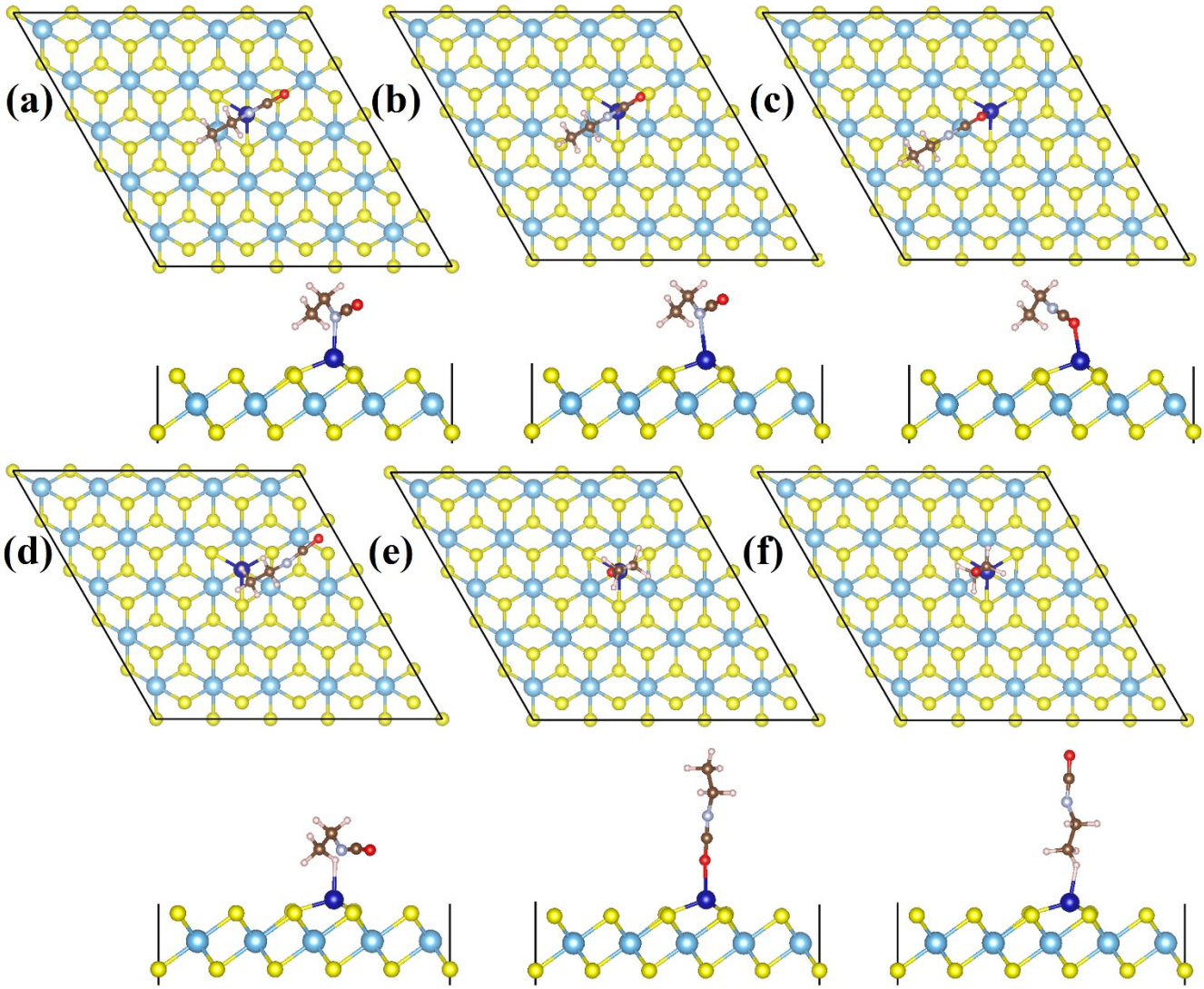

Figure S10: Top and side views of the final adsorption configurations of ethyl isocyanate (C_3H_5NO) on the Co-decorated-TiS_2 (Co-TiS_2) surface. Horizontal configurations include (a) N-atom, (b) C-atom, (c) O-atom, and (d) H-atom oriented parallel to the surface, while perpendicular configurations correspond to (e) H-atom and (f) O-atom oriented normal to the surface.

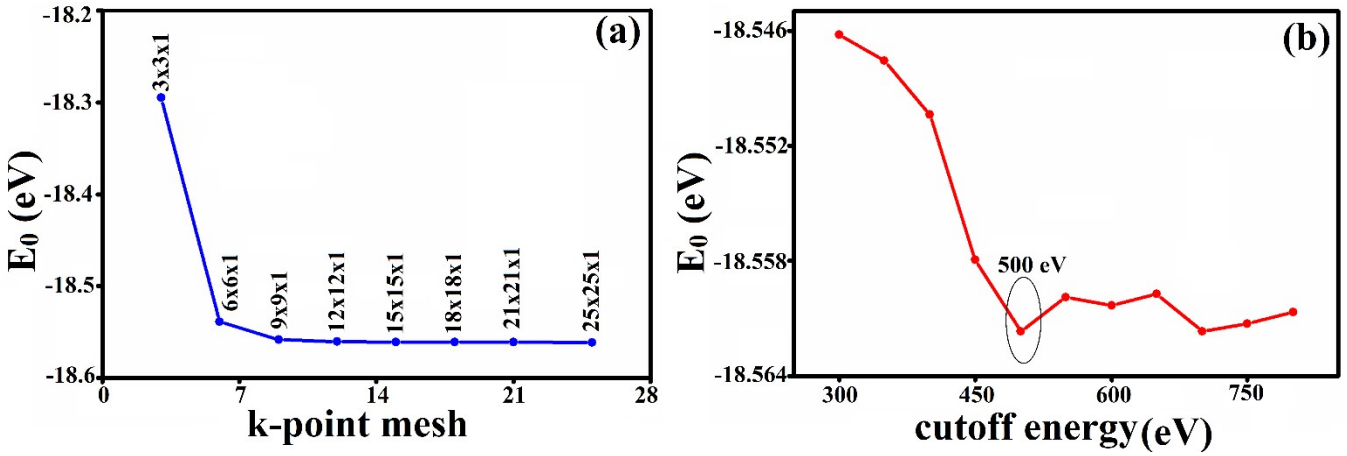

Figure S11: The convergence tests for (a) k-point grid and (b) cutoff energy

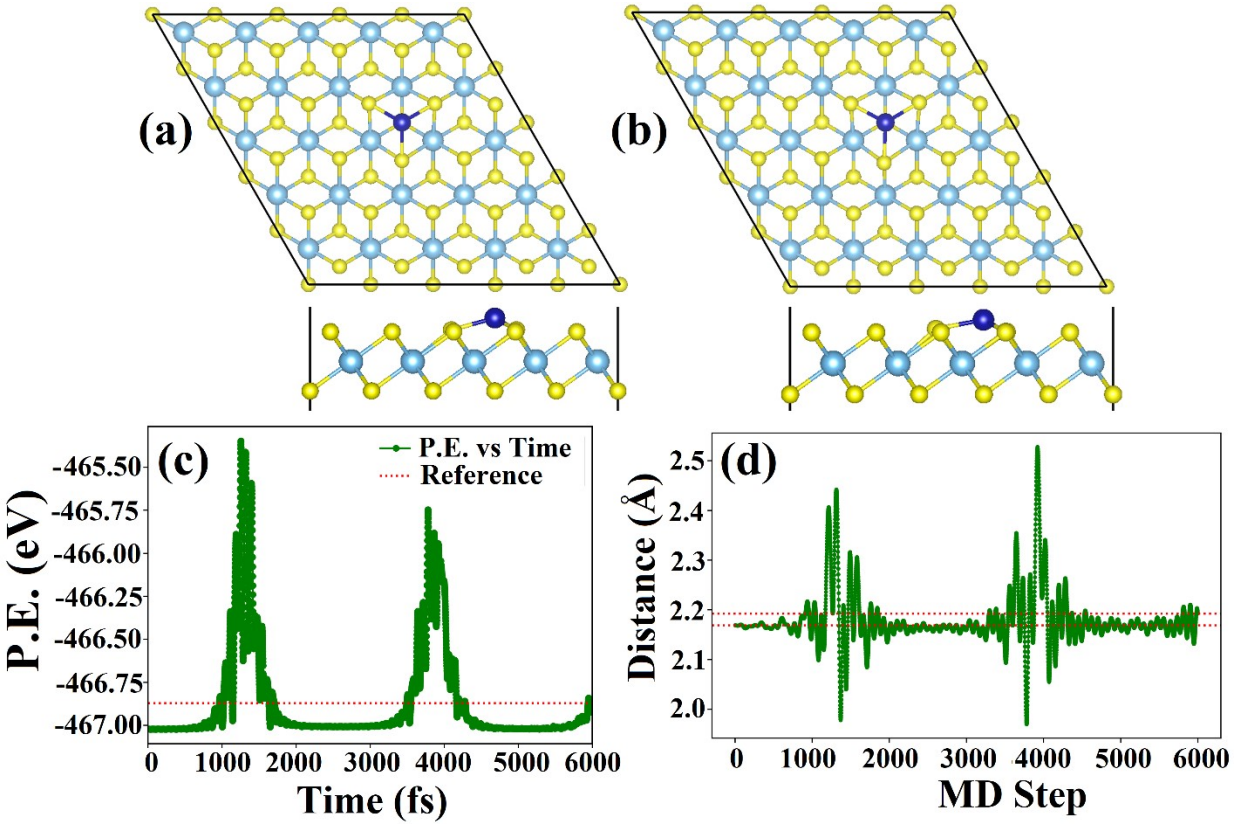

Figure S12: Top and side views of (a) initial structures of Co-TiS_2 at 0 K, (b) final structures of Co-TiS_2 at 300 K, (c) potential energy as a function of time step, and (d) displacement of Co atom as a function of MD step obtained from AIMD simulation for Co-TiS_2 at 300 K.