ELECTRONIC SUPPLEMENTARY INFORMATION
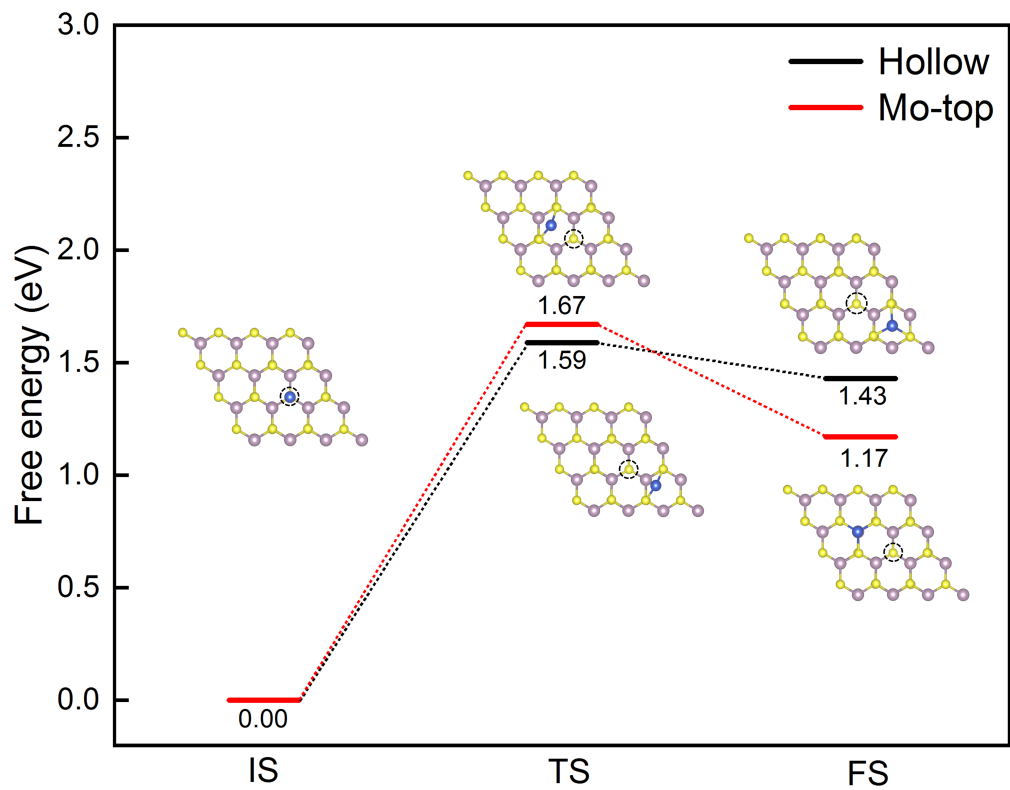
LIST OF FIGURES

FIG. S1. Diffusion pathways for migration of single Cu atom from sulfur vacancy to nearby Mo-top site (red-line) and hollow site (black-line).

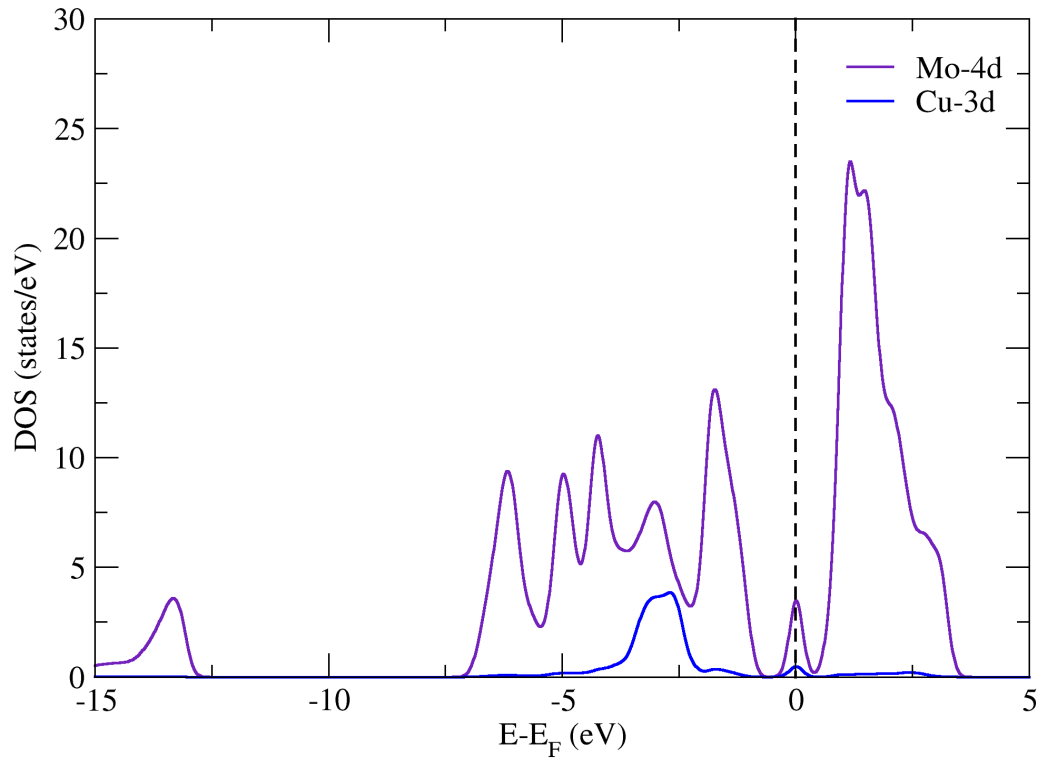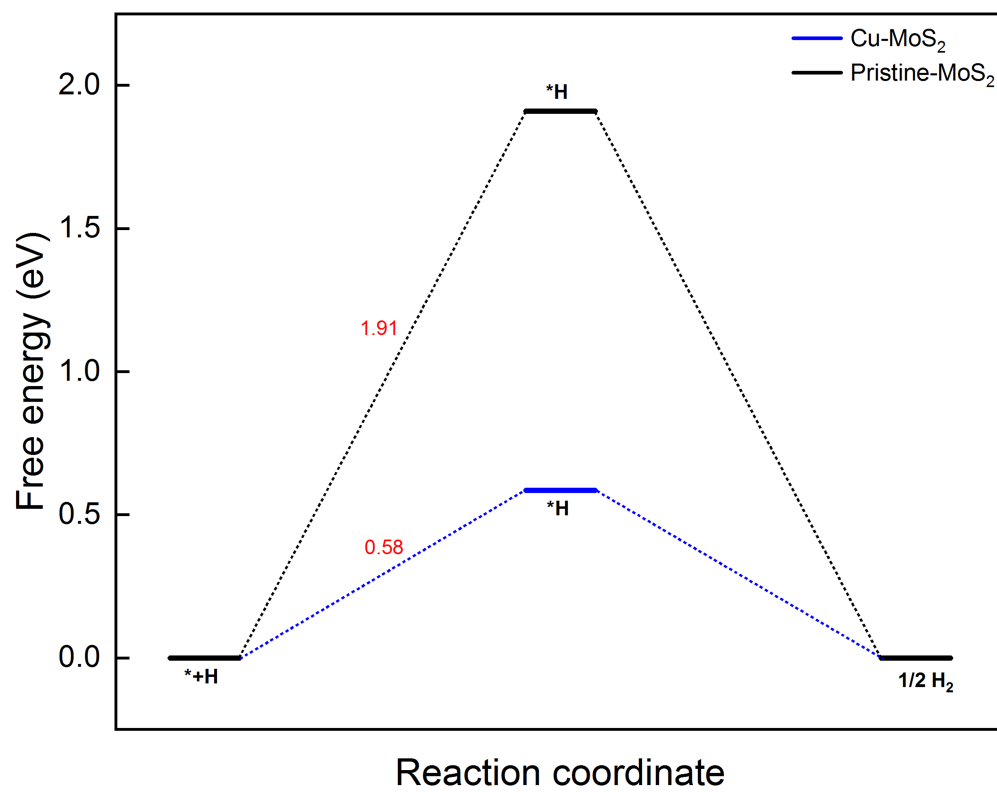FIG. S2. Projected density of states (PDOS) plot of Cu-MoS$_2$.

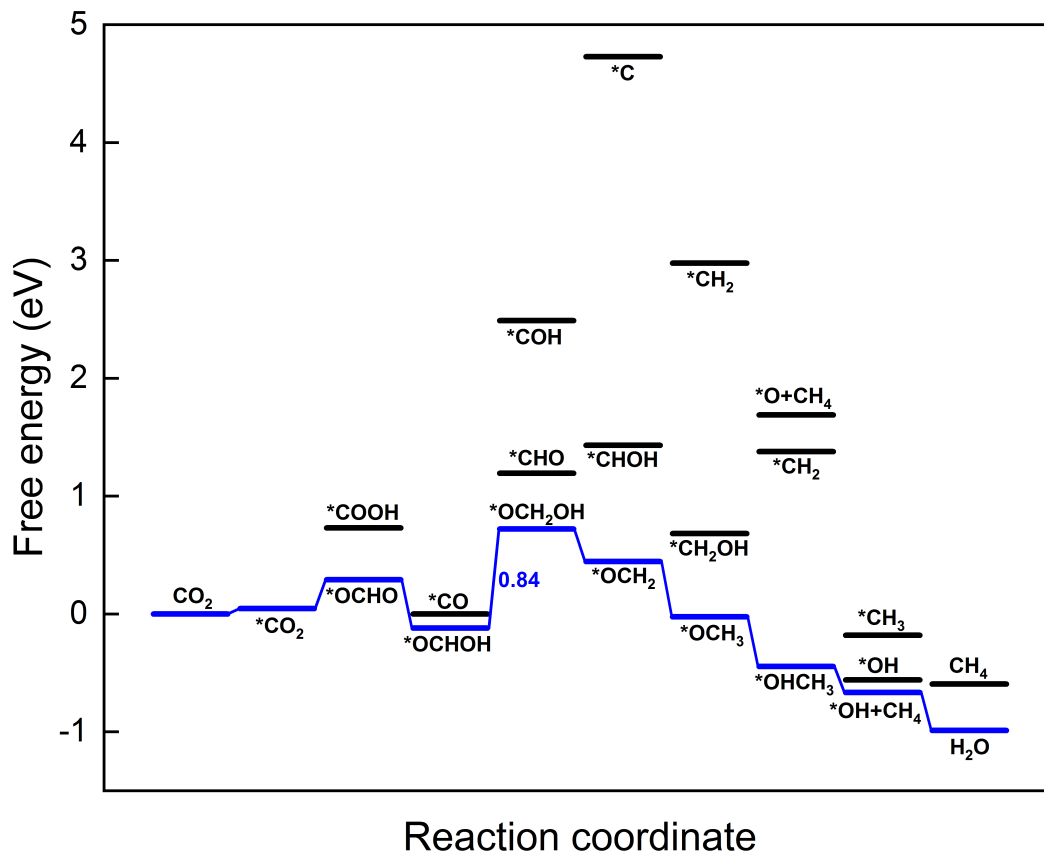FIG. S3. Gibbs free energy diagram of HER on Cu embedded MoS$_2$ monolayer.

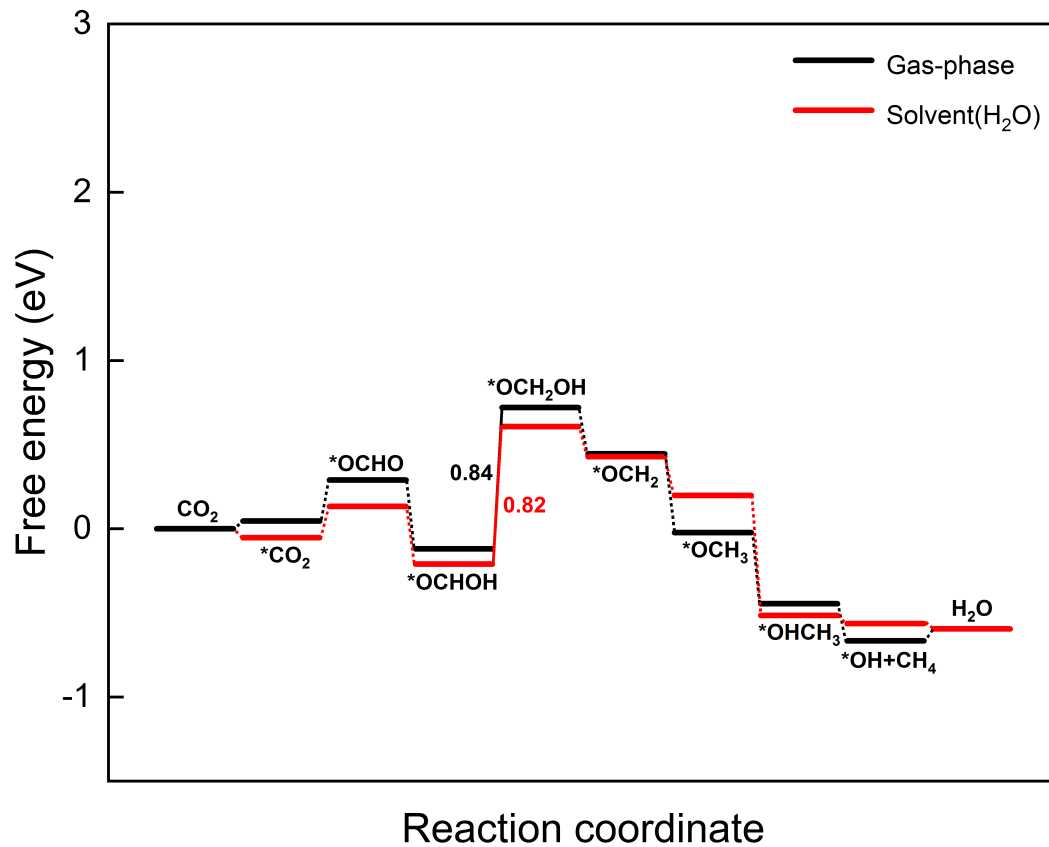FIG. S4. Gibbs free energy diagram of complete reaction path of CO_2RR on Cu-MoS_2 along C1 pathway.

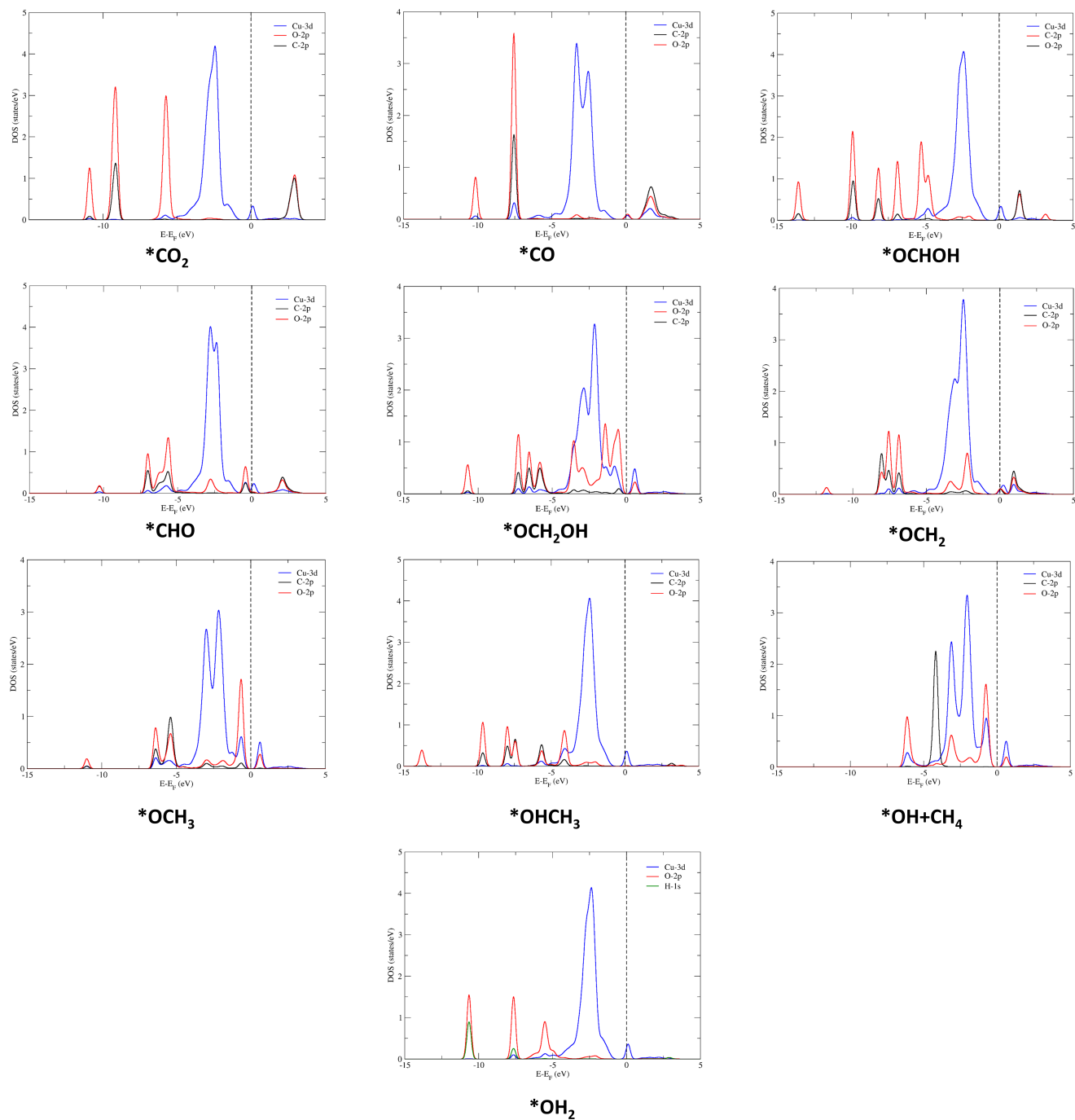FIG. S5. Gibbs free energy diagram for CO_2RR to CH_4 on Cu-MoS$_2$ with solvent effect.

FIG. S6. Projected density of states (PDOS) plot of various intermediates with Cu-3d on Cu-MoS$_2$ involved in CO$_2$RR process.
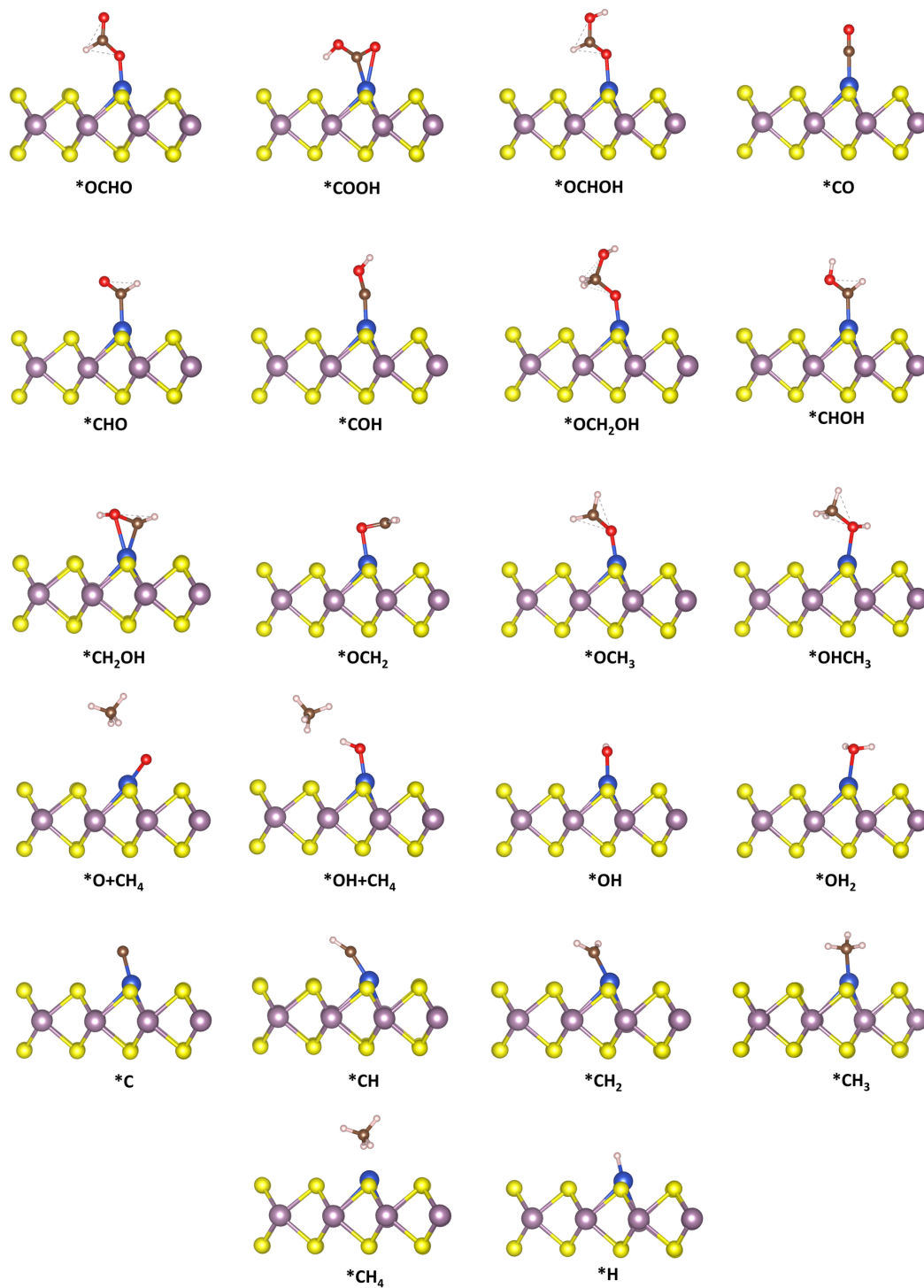
*OCHO ***COOH** ***OCHOH** ***CO**

*CHO ***COH** ***OCH$_2$OH** ***CHOH**

*CH$_2$OH ***OCH$_2$** ***OCH$_3$** ***OHCH$_3$**

*O+CH$_4$ ***OH+CH$_4$** ***OH** ***OH$_2$**

*C ***CH** ***CH$_2$** ***CH$_3$**

*CH$_4$ ***H**

FIG. S7. DFT-D3 optimized structures of various intermediates involved in CO_2RR on the Cu-MoS$_2$ monolayer.