

### Supporting Information

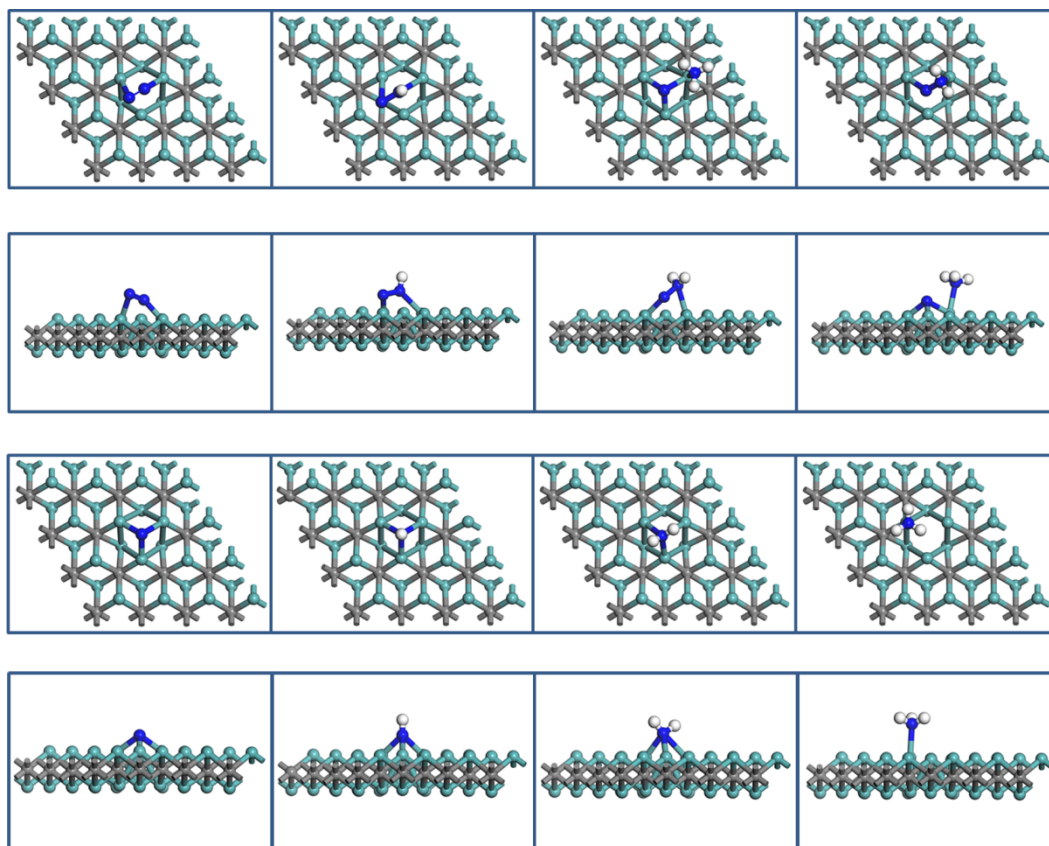


Figure S1. Optimized structures of reaction intermediate on  $V_C\text{-Mo}_2\text{C}$ .

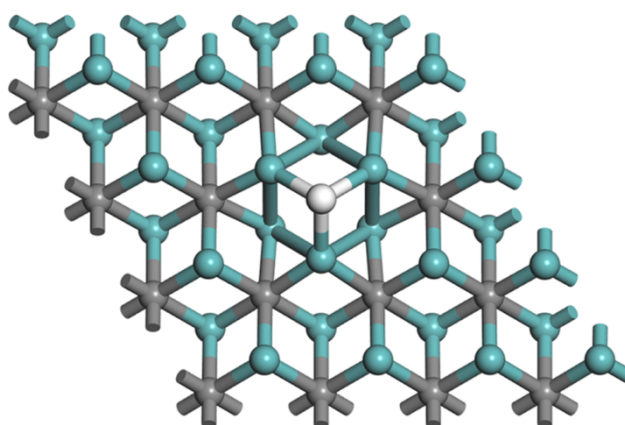


Figure S2. The optimized geometric structures of the adsorption of H on  $V_C\text{-Mo}_2\text{C}$ .

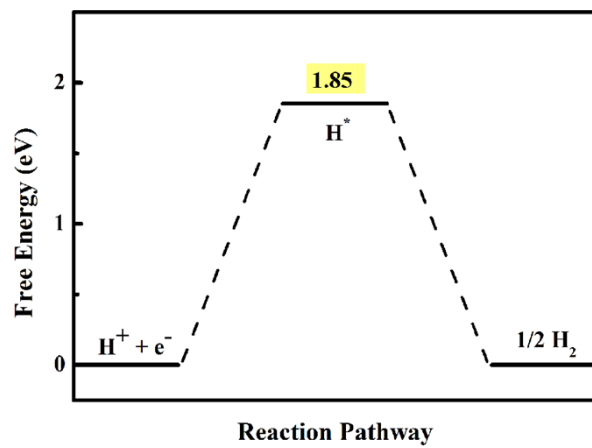


Figure S3. The Gibbs free energy diagram of HER on the V<sub>C</sub>-Mo<sub>2</sub>C.