

Supporting Information

Atomic and Molecular Adsorption on the Bi(111) Surface: Insights into Catalytic CO₂ Reduction

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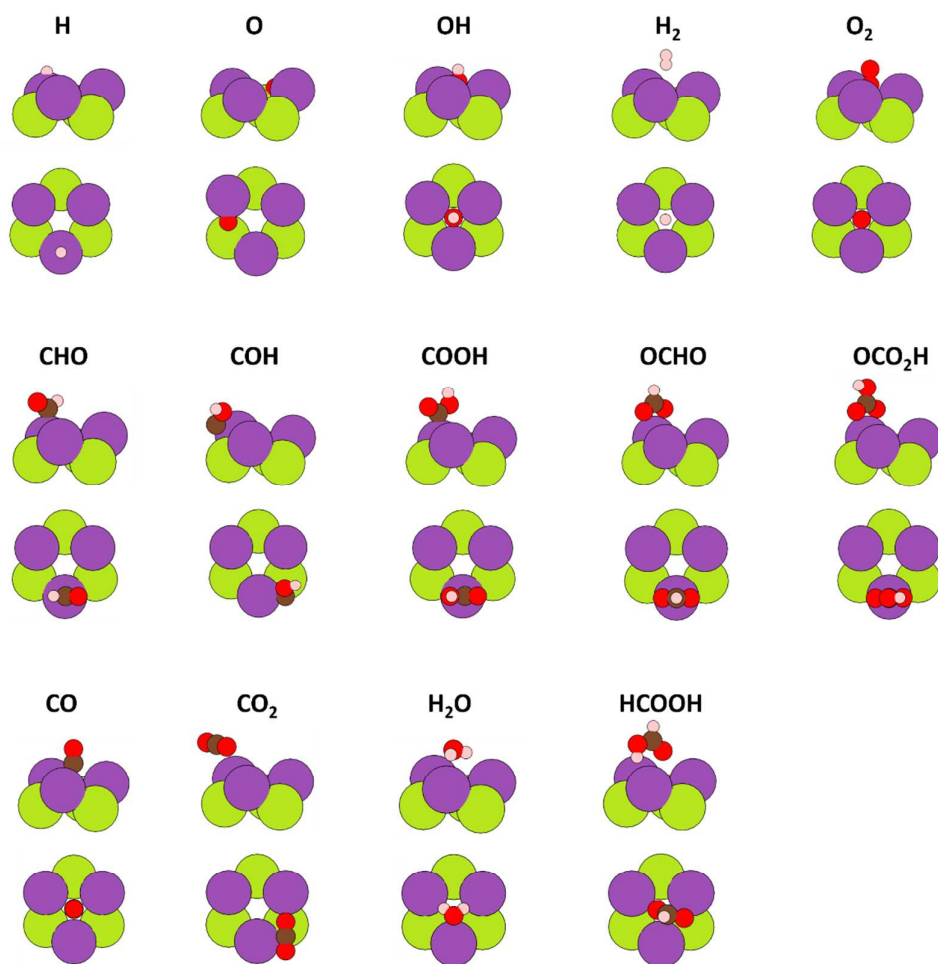


Figure S1. Geometry of the adsorbates: side view and top view.

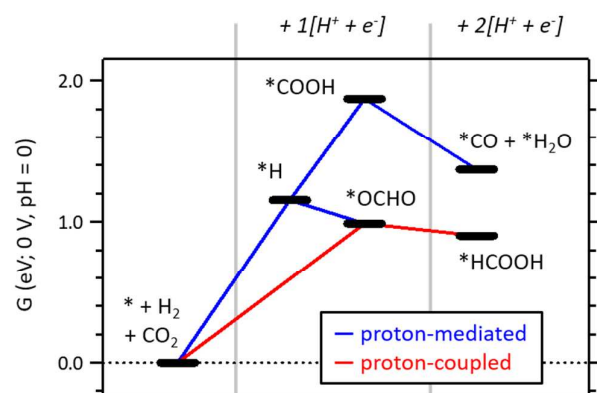


Figure S2. Free energy profiles for CO₂ reduction reaction on the Bi(111) surface (0 V vs. CHE, pH = 0).