

Article

Graphene Supported Tungsten Carbide as Catalyst for Electrochemical Reduction of CO₂

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In the submitted manuscript, we presented results for the electrochemical reduction of CO₂ on/by graphene-supported WC nanoparticles. For reasons of space/compactness, we did not present adsorbate snapshots in the main manuscript. They are provided in Figure SI.1 below. Details of the model catalyst structure used are as follows: The bulk crystal structure of WC was optimized using the described functional. A quasi-spherical 26 atom NP was cleaved from the center of the bulk crystal. The bottom of the WC nanoparticle (26 atoms) was saturated with excess C atoms to facilitate interaction/bonding with the graphene support. The structure was then optimized/relaxed to the same details provided in the manuscript. As can be seen in Fig SI.1, some carbon atoms on the lateral faces of the WC significantly relax to quasi-dimeric structures. Of the adsorbates discussed in this work, initial placement of atoms was tested over surface C atoms, surface W atoms, and surface C-C atoms. The FED energetics described in the manuscript main body use the lowest energy adsorption site/configuration for each species. The adsorbate snapshots in Figure S1 are for CO*, COH*, and COOH*, the lowest energy structure identified for each, respectively. Additional snapshot/structure files are available from the authors on request (email corresponding author RB Rankin) but due to ongoing work (that builds from/expands this manuscript results) are not currently included in this manuscript/SI.

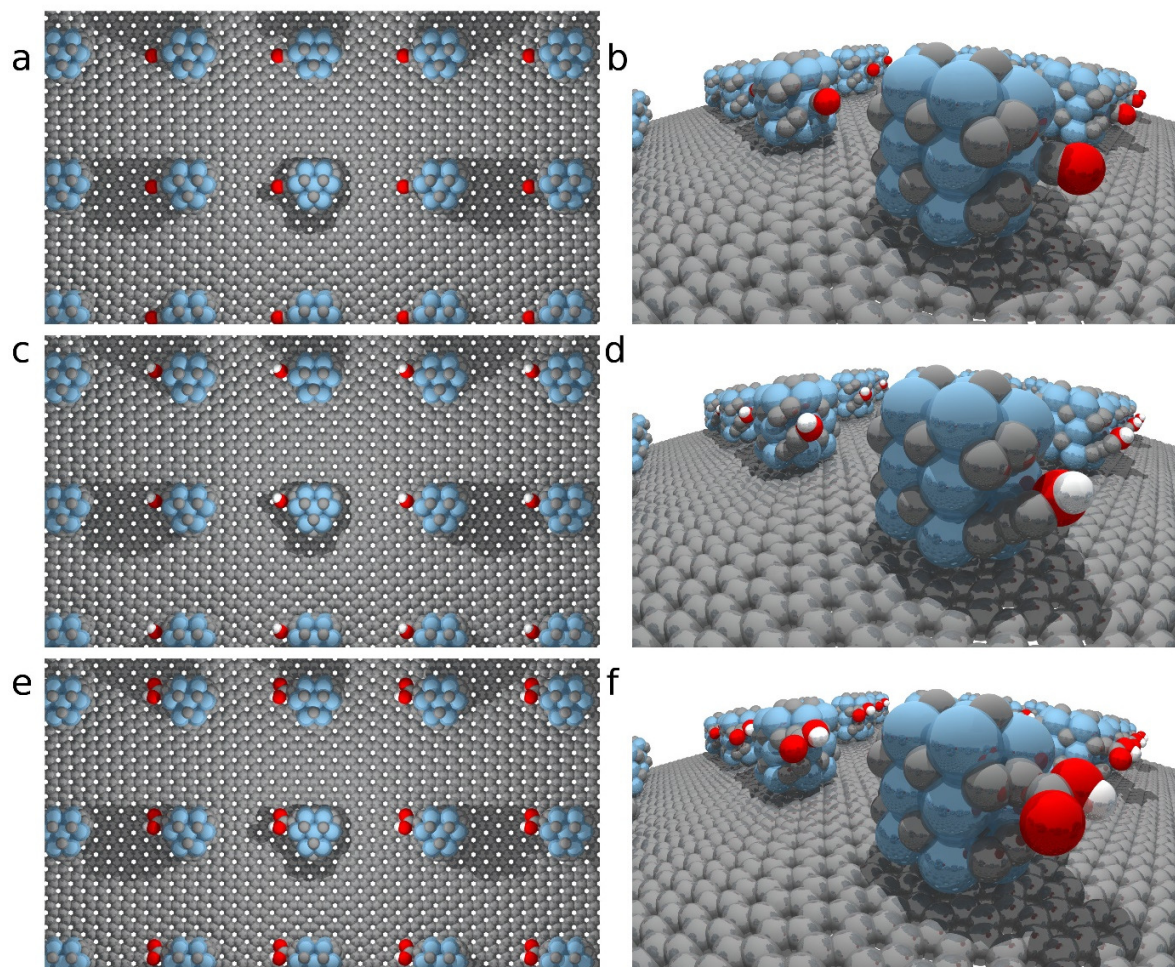


Figure S1: Adsorbate Snapshots for some key intermediates in the CO₂RR process reported in this manuscript on the WC/graphene hybrid catalyst/support system. Top-down views of CO*, COH*, and COOH*, given in panels **a**), **c**), and **e**), respectively. Side-on views of the same species, CO*, COH*, and COOH* given in panels **b**), **d**), and **f**), respectively. Color scheme: carbon (grey), tungsten (blue), oxygen (red), hydrogen (white).