Mo Single Atoms in the Cu(111) Surface as Improved Catalytic Active Centers for Deoxygenation Reactions

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Figure S1. Side (top) and top (bottom) views of the adsorption sites, together with the adsorption energies, for the studied reactants as adsorbed on Cu(111) and Mo(011) surface. Cu and Mo atoms are represented as blue and pink spheres, plus white, green, and red spheres denote molecular H, C, and O atoms, respectively.

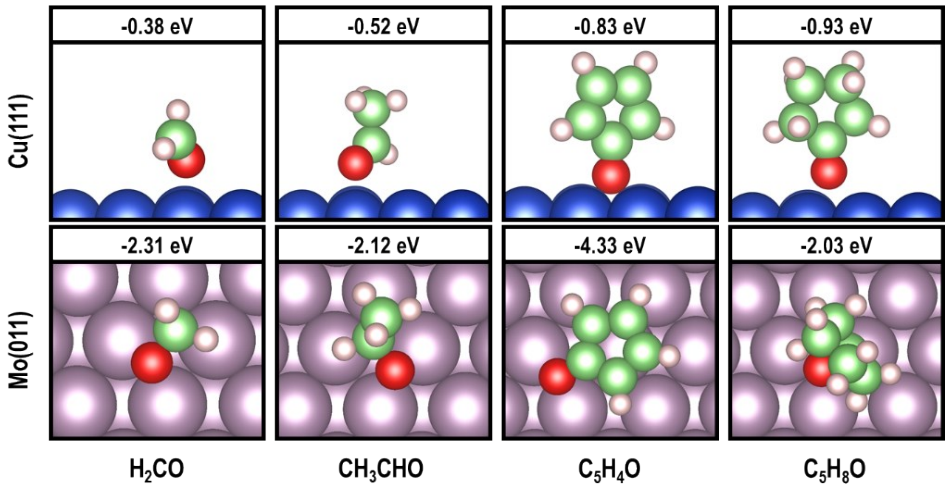

Figure S2. Top views of the adsorption sites and adsorption energies for the studied isolated deoxygenation products on Cu(111) and Mo(011) surfaces. Color code as in Figure S1.

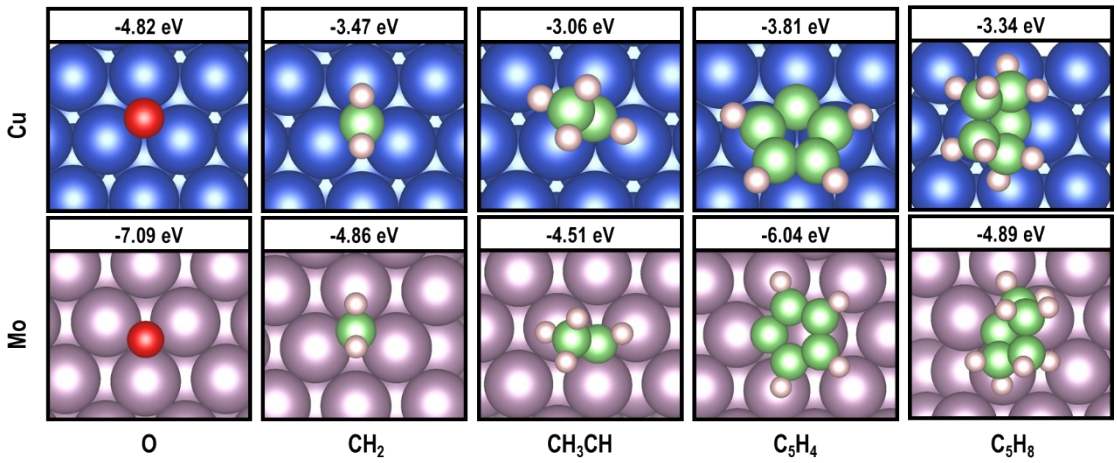

Figure S3. Top views of the adsorption sites and adsorption energies for the co-adsorbed products of the deoxygenation reactions as studied on Cu(111) and Mo(011) surfaces. Color code as in Figure S1.

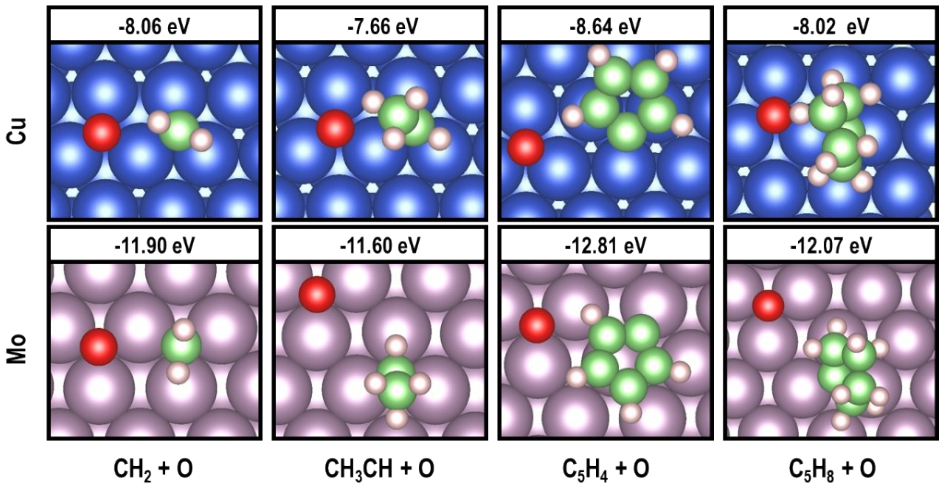

Figure S4. Top views of the adsorption sites and reaction energy barriers for the transition states of the deoxygenation reactions as studied on the Cu(111) and Mo(011) surfaces. Color code as in Figure S1.

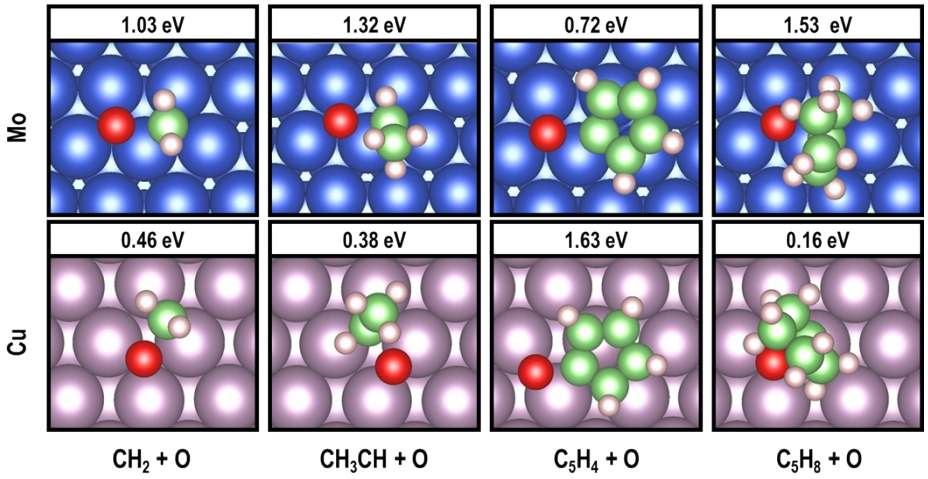

Figure S5. Top views of the adsorption sites and adsorption energies for the reactants adsorbed on either a supported- or a doped-Mo SAC. Color code as in Figure S1.

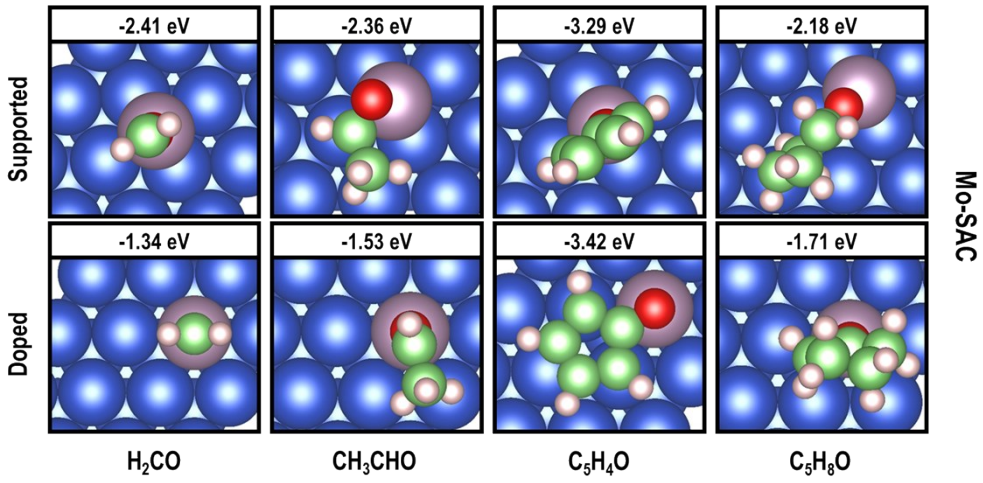

Figure S6. Top views of the adsorption sites and adsorption energies for the isolated reaction products on either a supported- or a doped-Mo SAC. Color code as in Figure S1.

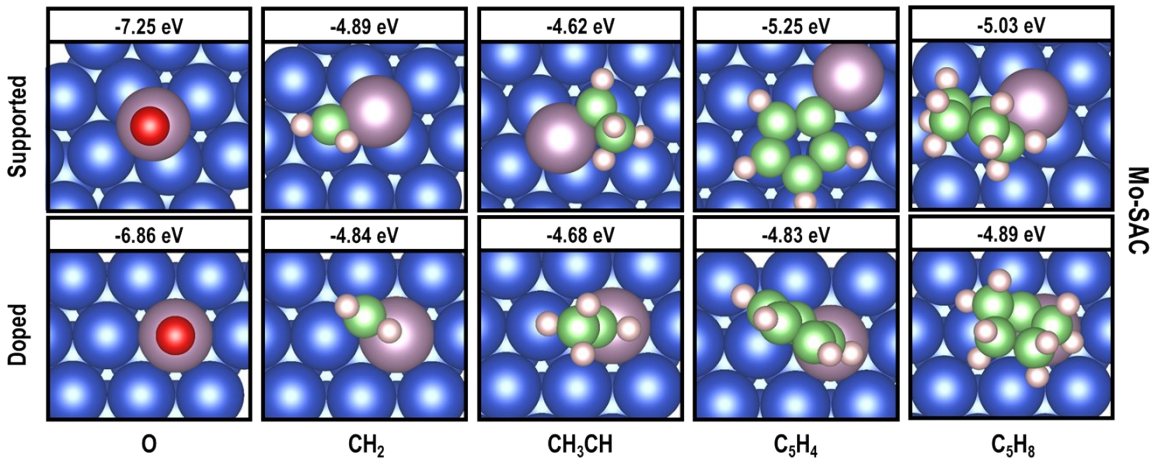

Figure S7. Top views of the adsorption sites and adsorption energies for the co-adsorbed products of the deoxygenation reactions on either a supported- or a doped-Mo SAC. Color code as in Figure S1.

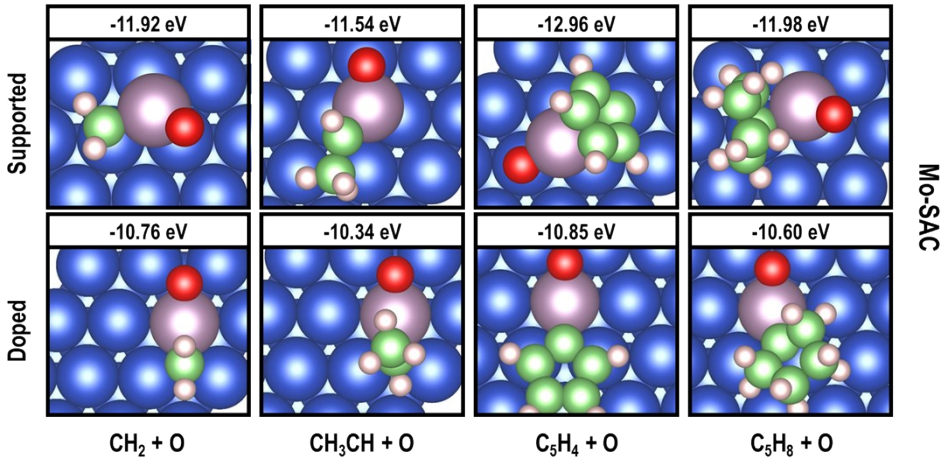

Figure S8. Top views of the adsorption sites and reaction energy barriers for the obtained transition states of the studied deoxygenation reactions explored on either a supported- or a doped-Mo SAC. Color code as in Figure S1.