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Article

Study of the Glycerol Hydrogenolysis Reaction on Cu, Cu–Zn, and Cu–ZnO Clusters

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ABSTRACT: Quantum chemistry calculations have been performed to access the efficacy of Cu-based catalysts in various mechanistic steps of the glycerol hydrogenolysis reaction. Calculations are first performed for reactants in the gas phase (noncatalyzed system) and reactants in the gas phase with a 3-atom Cu cluster (catalyzed system). We demonstrate that the glycerol to ethylene glycol conversion is preferred in the noncatalyzed system but glycerol conversion to 1,2-propanediol via the 2-acetol intermediate is preferred in the catalyzed system. We next analyze the adsorption energies of the reactant and product species involved in the glycerol to 1,2-PDO reaction on an 8-atom Cu cluster and Cu cluster doped with a Zn atom or a ZnO molecule. Finally, we study the effects of Zn or ZnO doping on the activation barriers of the two steps of the glycerol to 1,2-PDO reaction.