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Atomic structures and energetics of methanol and its reaction intermediates on the ZnO(0001) surface : A first-principles study
KATAWUT CHUASIRIPATTANA, OLIVER WARSCHKOW, University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHY STAMPFL, University of Sydney — Methanol (CH_3OH) is widely used in various chemical synthesis, and in particular it is predicted to be one of the next generation of renewable energy sources as a fuel for fuel cells. Industrially, methanol is mass produced by Al_2O_3-supported Cu/ZnO catalysts. However, the role of ZnO in the methanol systhesis is still unclear. To provide a better understanding of the mechanisms underlying this process, we present first-principles total- energy calculations of the methanol molecule and its reaction intermediates on the ZnO(0001) surface. A detailed characterization of atomic geometries and associated energetics is presented. The reaction intermediates we consider are CH_3O, CH_2O, CH_3, HCOOH, HCOO, HCO, H_2O, CO_2, CO, OH and H. These intermediate species are reported from experimental studies to be present during methanol decomposition on the ZnO(0001) surface. We also analyse the vibrational frequencies of each of the adsorbed fragments. The information obtained will be used for investigating the surface chemical reactions of associated with methanol synthesis over the ZnO surface.

Katawut Chuasiripattana
University of Sydney

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