Single Paladium catalyst supported on reducible oxide for hydrogen generation from HCOOH: An ab initio DFT study

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Formic acid (HCOOH) has continued to receive attention from audiences because of its vital role in the storage and transport of Hydrogen (H2), coupled with its non-toxic nature. Depending on the reaction conditions and catalyst involve, HCOOH may undergo dehydrogenation or dehydration to produce H2 and/or CO. H2 is a zero-emission energy and it is the desired product expected from HCOOH decomposition. However, CO which often cause catalyst deactivation may be generated if the dehydration route is favored. Several experimental and theoretical literatures have shown that Pd-based catalyst is the most active catalyst for hydrogen production via HCOOH decomposition, although the cost is high. Incorporation of secondary metals, although have shown to improve its activity, notwithstanding, this technique still results in high use of active metal catalyst. The use of single metal cluster embedded on various supports such as reducible and irreducible metal oxide is a promising techniques that can aid the proper utilization of active metals. In this report, single Pd cluster (Pd_1) incorporated on various metal oxide supports (MgO, TiO2, ZrO2) was used to investigate HCOOH decomposition.