The First-Principles approach to the effects of shell thickness in enhancing productivity and selectivity for HCOOH decomposition on the bimetallic Ag-Pd core-shell catalyst

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The oxidation of small organic molecules has been widely studied owing to fundamental interest and relevance to fuel cell technology. Among these molecules, formic acid is an excellent in situ source of hydrogen for fuel cells, for it offers high energy density and remains as liquid at standard temperature and pressure. So far, there has been a lack of reports regarding the formic acid decomposition mechanism on a bimetallic heterogeneous catalyst. In this study, We, hereby, report the decomposition mechanism and electronic properties of HCOOH when using Ag-Pd core-shell catalyst. The formic acid decomposition mechanism is investigated using Climbing Nudged image Elastic Band Method (CiNEB) and reaction energies. We find that strain and ligand effects in a heterogeneous bimetallic catalyst lead to a drastic change in the electronic and chemical properties of the top surface. In summary, the thinnest Pd shell catalyst stimulates hydrogen production from formic acid decomposition at room temperature and this result provides possibilities of the development of fuel cell devices.