The First-Principles approach to the formic acid decomposition mechanism on a Ag-Pd core-shell catalyst

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Formic acid is an excellent *in situ* source of hydrogen for fuel cells, for it offers high energy density and remains as a liquid at standard temperature and pressure. So far, there has been a lack of reports regarding the formic acid decomposition mechanism on a bimetallic heterogenous catalyst. we, hereby, report for the first time decomposition mechanism of formic acid and electronic properties of the top layer of Ag-Pd core-shell catalyst. The formic acid decomposition mechanism is investigated using a climibing nudged image elastic band method (CiNEB) and reaction energies. We find that the ligand effect in a heterogeneous catalyst plays important role in determining formic acid decomposition rather than the strain effect. In particular, the thinnest Pd shell catalyst boosts the hydrogen production from formic acid decomposition at room temperature and this result provides possibilities for the development of fuel cell devices.