In silico design of alloy catalyst materials for formic acid decomposition

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Density functional theory calculations are employed to investigate the energetics of formic acid decomposition on Ag, Cu, Pd, Pt and Rh surfaces. The study is also extended to other transition metal surfaces by utilizing the linear relations obtained when the adsorption energies of the reaction species are scaled to CO and OH adsorption energies. By incorporating the scaling relations in a microkinetic model, the kinetics of formic acid decomposition are mapped as functions of CO and OH adsorption energies. The variations in catalytic activity and selectivity from one metal surface to another obtained in silico in this study are in good agreement with those obtained experimentally. Finally, we illustrate a method for screening potentially interesting alloy catalyst materials based on the calculated catalytic activities of transition metal elements and the interpolation concept of adsorption energy.