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Hydrogen production from methanol on transition metals: A study of thermodynamics and kinetics on subnanometer clusters FAISAL MEHMOOD, JEFFERY P. GREELEY, PETER ZAPOL, LARRY A. CURTISS, Argonne National Laboratory — The mechanistic studies of Pd-based catalysts and its interaction with methanol have attracted huge attention because of the possibility of using methanol as an on-board source of hydrogen for fuel cells. Stabilizing subnanometer metal clusters is a challenging process that has exhibited novel catalytic properties for various industrially important reactions such as production of hydrogen from hydrogen-rich molecules. One such reaction is methanol decomposition that was modeled by applying DFT methods on metal clusters. The thermodynamics and kinetics of three decomposition routes involving C-O, C-H and O-H scission were investigated; activation energy barriers were determined with the nudged elastic band method on Pd clusters with a comparison to Co and Cu clusters. A detailed analysis of the PES for methanol decomposition shows C-O activation to be the least favorable step on all three metal clusters. However we find activation to be $\sim$0.30 eV smaller on Co cluster. In addition, estimated thermodynamical data for a large number of transition metals has been generated from linear correlations constructed from the binding energies of Pd, Cu and Co to broaden our understanding of the role such metal clusters can play as catalyst for such reactions.

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