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A density functional theory study of structure-property relationships for Pt-Ni alloy catalysts LIANG CAO, Department of Physics and Astronomy, Johns Hopkins Univesity, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — The ORR (Oxygen Reduction Reaction) is an important reaction in devices such as metal-air batteries and PEMFCs (Polymer Electrolyte Membrane fuel cells). Pure Pt is one of the most successful electrode catalysts for this key reaction. However, due to its expense, numerous efforts have been made to find a new catalysis system based on Pt bimetallic alloys, in which Pt is partially replaced by less expensive metals, such as Ni, Co and Fe. Experimental and theoretical works have shown that Pt3Ni alloys have a higher ORR activity than pure Pt. In order to investigate the enhanced catalytic activity, cluster expansions corresponding to a simplified 9-layer Pt-Ni slab model are built to accurately and quickly predict the energies of surfaces as a function of atomic order. With the help of this model, we can study systematically the atomic structure and the surface geometry of Pt3Ni surface system at a variety of temperature and chemical environments, and we can calculate the adsorption binding energies of O, OH and H on both equilibrium and non-equilibrium Pt-Ni(111) surfaces. Also, we can investigate the effects of off-stoichiometry on surface by searching for stable ground states under different concentrations.

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