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Thermodynamics of alloyed nanoparticles for hydrogen evolution reaction including configurational and adsorbate effects[1] LIN-LIN WANG, Ames Laboratory, U.S. Department of Energy, Ames, IA 50011, TECK L. TAN, Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore 138632, Singapore, DUANE D. JOHNSON, Ames Laboratory, U.S. Department of Energy, Ames, IA 50011; Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — Changes in the chemical configuration of alloyed nanoparticle (NP) catalysts induced by adsorbates under working conditions are crucial to understand and design NP functionality. We extend the cluster expansion method to predict the configurational thermodynamics of alloyed NPs on equal footing with adsorbate thermodynamics based on density functional theory data. Exemplified with alloyed PdPt NPs having H-coverage up to a full layer, we describe both the configurational and adsorbate thermodynamics behavior simultaneously across the entire range of NP composition and H-coverage to obtain the H-adsorption isotherms and simulated cyclic voltammetry for hydrogen evolution reaction.

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