Abstract Submitted
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**First-principles configurational thermodynamics of alloyed nanoparticles with adsorbates**[1] LIN-LIN WANG, Ames Laboratory, U.S. Department of Energy, TECK L. TAN, Institute of High Performance Computing, Agency for Science Technology and Research, Singapore, DUANE D. JOHNSON, Department of Materials Science and Engineering, Iowa State University — Transition-metal, alloyed nanoparticles (NPs) are key components in current and emerging energy technologies because they are found to improve catalytic activity and selectivity for many energy-conversion processes. However, thermodynamic investigations of the compositional profile of alloyed nanoparticles, which determines their catalytic properties, have been limited mostly to NP core-shell preference without the presence of adsorbates. Here, by extending cluster expansion methods to treat both alloyed nanoparticles and adsorbates, we study the configurational thermodynamics of bimetallic NPs under chemically reactive conditions, using databases from density functional theory calculations. With a few examples, we show that such simulations can provide information needed for rational design of NP catalysts.

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