Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Configurational thermodynamics of alloyed nanoparticles: a first-principles cluster expansion study[1] LIN-LIN WANG, Division of Materials Science and Engineering, Ames Laboratory, DUANE D. JOHNSON, Division of Materials Science and Engineering, Ames Laboratory and Iowa State University — Transition-metal, alloyed core-shell nanoparticles (NPs) continue to be studied as heterogeneous catalysts because they are found to improve catalytic activity and selectivity for many energy-conversion processes. However, thermodynamic investigations have been limited mostly to NP core-shell preference, rather than both geometric structure and its chemical decoration. Here, by extending cluster expansion methods to treat alloyed nanoparticles, we study the configurational thermodynamics of bimetallic NPs, using databases from density functional theory calculations. We find that the interplay between the ordering tendency and the core-shell segregation tendency can induce site-specific preferences around the NP, as we exemplify, e.g., in AgAu. Such simulations will provide information needed for further understanding of the structure-function relationships in NP catalysis.

[1]Supported by the DOE/BES under DE-FG02-03ER15476 (Catalysis) and DE-AC02-07CH11358 at the Ames Laboratory operated by Iowa State University

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Date submitted: 11 Nov 2011 Electronic form version 1.4