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Universal Behavior of Core-Shell Preferences in Transition-Metal Nanoparticles[1] LIN-LIN WANG, DUANE D. JOHNSON, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Transition-metal, core-shell nanoparticles are becoming ubiquitous from (electro-) catalysis to biomedical applications, due to control of size, performance, biocompatibility, and cost. We investigate 66 binary core-shell nanoparticle systems (groups 8 to 11 in the periodic table) using density functional theory (DFT) and systematically explore their segregation energies to determine core-shell preferences. We find that core-shell preferences are described by two simple factors: (1) cohesive energy (related to vapor pressure) and (2) atomic size (quantified by Wigner-Seitz radius). Core-shell preferences determined from DFT segregation energies agree with all available observations, and predict others, which can be used for design purposes. We then provide a universal description of core-shell preference via tight-binding band-energy differences that (i) quantitatively reproduces the DFT segregation energies and (ii) confirms the electronic origins for core-shell behavior.

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