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Energetic and structural analysis of 102-atom Pd-Pt nanoparticles[1] RAFAEL PACHECO-CONTRERAS, DIFUS, ALVARO ARTEAGA-GUERRERO, DFUS, DORA JULIA BORBON-GONZALEZ, Dept de Matematicas, UNISON, ALVARO POSADA-AMARILLAS, DIFUS, J. CHRISTIAN SCHOEN, Max Planck Institute for Solid State Research, ROY L. JOHNSTON, School of Chemistry, University of Birmingham — We present an extensive study of the structural and energetic changes of 102-atom Pd_mPt_{102-m} nanoparticles as a function of composition m, where the interatomic interactions are modeled with the many-body Gupta potential. The minimum energy structures are obtained through a genetic algorithm. The excess energy is calculated, as well as the pair distribution function $g(r)$. The radial distribution of the atoms is computed for each composition; the result indicates a multi-layer segregation for some compositions, with a shell growth sequence as follows: a core with a small number of Pd atoms is followed by an intermediate shell of Pt atoms and the external shell consists of Pd atoms. A region where Pd and Pt atoms are mixed is observed between the outermost and intermediate shells. Furthermore, the pure Pd_{102} and Pt_{102} nanoparticles have the same structure, while a variety of different structures are observed for the bimetallic clusters.

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