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Revised Basin Hopping Monte Carlo Algorithm Applied for Nanoparticles[1] JUAREZ L. F. DA SILVA, Institute of Chemistry of Sao Carlos, USP, Brazil, GUSTAVO G. RONDINA, Institute of Physics of Sao Carlos, USP, Brazil — The Basin Hopping Monte Carlo (BHMC) algorithm has been very successful in obtaining the atomic structure of nanoparticles (NPs), however, its application for unbiased randomly initialized NPs have been restricted to few hundreds atoms employing empirical pair-potentials (EPP) and for small clusters employing first-principles interacting potentials based on density functional theory (DFT). In this talk, we will present our suggestions for bringing improvements to the the BHMC algorithm, which successfully extend its application for relatively large systems employing EPP and DFT potenticals. Using our implementation from scratch, we have found all the reported putative minimum energy configurations for Lennard-Jones and Sutton-Chen EPPs (N = 2 - 147, 200, 250, 300, ..., 1000). We addressed also binary systems described by the Lennard-Jones or Sutton-Chen empirical potentials, and excellent results have been obtained. Finally, our revised BHMC implementation was combined with DFT potentials (FHI-AIMS), which was employed to study the atomic structure of Al clusters from 2 - 55 atoms in the neutral and charged states. Thus, our results indicate the our suggestions provide an important contribution to improve the quality of the BHMC results employing EPP or DFT potentials.

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