Title:	Electrostatics-Assisted Building-Up Procedure for Capturing Energy Minima of Metal Clusters: Test Case of Agn Clusters
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Abstract:	Global geometry optimization of metal clusters is an important problem in nanophysics. The starting geometries of the clusters generated with empirical or other model potentials are generally optimized further by density functional theory (DFT)-based energy minimization. For this purpose, several algorithms such as simulated annealing, genetic algorithms, basin hopping, etc. are used. Our building-up procedure generates putative lower-energy structures of metal (M) clusters, Mn+1, Mn+2, etc., by anchoring one or more metal atoms in the vicinity of the minima of the molecular electrostatic potential (MESP) of Mn. Here, we report an application of this method to Agn clusters, for 5 ≤ n ≤ 20, followed up by DFT-based geometry optimization, generating several lower-energy structures than those reported in the literature. New low-energy isomers are obtained by applying the same procedure to the test case of mixed-metal clusters, NinAgm, for n + m = 4 and 5. In conclusion, our MESP-based building-up procedure offers a new general methodology for generating lower-energy geometries of metal clusters.
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