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Park, Y.H., Hijazi, I.

Determination of transitional size of metal clusters
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Abstract
We investigated the transitional size of metal clusters where the electronic effect and the size effect on the ground state structure become weaker. Identification of a transitional size cluster provides the means to efficiently determine the ground state structure of large clusters using density functional theory. Beyond the critical size of clusters, geometrical effects become important and the putative global minimum obtained from an empirical method can be used to determine the true ground state structure where the size effect on structures is less significant. We identified the lowest-energy structure using a first principles method in combination with the global search algorithm. We then used the similarity function to quantify structural difference and similarity between the global minimum obtained from an empirical method and the true ground state structure. Two structures become similar beyond a certain critical size. To investigate low-lying structures of metal clusters, we used a Monte Carlo simulated annealing method which employs the Aggregate-Volume-Bias Monte Carlo (AVBMC) algorithm. Incorporated in the Monte Carlo method is an Embedded Atom Method (EAM) potential developed by the authors. Copyright © 2013 by ASME.

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