Metallic behavior of Pd atomic clusters

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Abstract

We report a study of the nonmetal–metal transition of free-standing PdN clusters ($2 \leq N \leq 21$) carried out through two different theoretical approaches that are extensively employed in electronic structure calculations: a semi-empirical tight-binding (TB) model and an *ab initio* DFT pseudopotential model. The calculated critical size for the metallic transition decreases rapidly with the temperature and an oscillatory dependence with the cluster size is obtained, particularly in the DFT approach. The TB model describes the metallic behavior for cluster sizes beyond $N \approx 12$ well. Our obtained critical size at room temperature is of the order of the experimental estimation.