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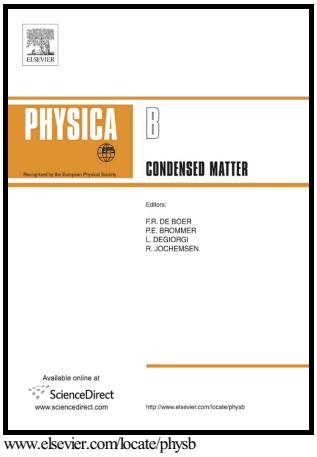

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Cluster perturbation theory for calculation of electronic properties of ensembles of metal nanoclusters

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Abstract

The method is developed for calculation of electronic properties of an ensemble of metal nanoclusters with the use of cluster perturbation theory. This method is applied to the system of gold nanoclusters. The Green's function of single nanocluster is obtained by *ab initio* calculations within the framework of the density functional theory, and then is used in Dyson equation to group nanoclusters together and to compute the Green's function as well as the electron density of states of the whole ensemble. The transition from insulator state of a single nanocluster to metallic state of bulk gold is observed.

1. Introduction

Ensembles of metal nanoclusters are characterized by unique physical and chemical properties. These properties differ from the properties of both bulk metals and individual atoms, and currently are studied with particular intensity due to numerous potential applications in physics, chemistry, and engineering. Existing universally accepted numerical methods of studying the electronic structure of many-body systems, such as density functional theory (DFT) and quantum Monte Carlo algorithms (QMC), encounter serious difficulties associated with the need to take into account a large number of elements of a system, since individual nanoclusters of the ensemble do not form an ordered structure as a whole. Therefore, for correct simulation of such ensembles it is necessary to consider systems containing hundreds

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