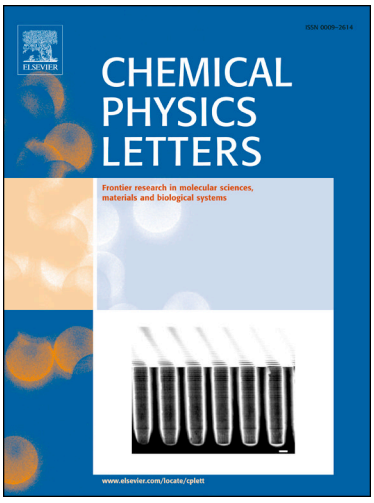

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An algorithm to use higher order invariants for modelling potential energy surface of nanoclusters

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Abstract

In order to fit potential energy surface (PES) of gold nanoclusters, we have integrated bispectrum features with artificial neural network (ANN) learning technique in this work. We have also devised an algorithm for selecting the frequencies that need to be coupled for extracting the phase information between different frequency bands. We have found that higher order invariant like bispectrum is highly efficient in exploring the PES as compared to other invariants. The sensitivity of bispectrum can also be exploited in acting as an order parameter for calculating many thermodynamic properties of nanoclusters.

Keywords: descriptor, artificial neural networks, molecular dynamics simulations, gold nanoclusters, power spectrum, bispectrum

1. Introduction

Metal nanoclusters consisting of small number of atoms and size typically less than 2 nm, have evoked considerable attention due to their highly reactive surface[1]. High reactive surface in nanoclusters are due to presence of large number of surface atoms. For understanding unique properties such as high reactive surface, it is essential to explore the underlying PES of the metal nanocluster. Construction of PES for a metal nanocluster using first principle studies is computationally expensive since exploring different minima using molecular dynamics (MD) simulations or global optimizations is very time consuming. So, to explore the PES we have to use methods which have an accuracy of first principles study and which are easy to compute. Focus of our study is to obtain the structure and properties of gold nanoclusters since they find various applications in biomedical sciences[3], plasmonics[3], drug delivery[4] among many others. In the current work, we have constructed the PES for a wide range of Au_n (n=30-147) nanoclusters.