Global Optimization of Atomic Clusters: A Soft Computing Perspective

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Abstract

Geometry optimization of chemical systems like atomic clusters becomes a daunting task because of the large size of the search space and the possibility of getting stuck in a local minimum on the potential energy surface.

Determination of global minimum energy structure needs the gradient and Hessian matrices to be calculated at each stage and with no guarantee of locating the global minimum. Various soft computing techniques may be made use of, bypassing this hassle. We present methods like particle swarm optimization combined with density functional theory, atom centered density matrix propagation and convolutional neural network and also a firefly algorithm for global optimization of atomic clusters. We highlight their efficiency and accuracy by considering different metallic and non-metallic clusters as prototype examples. A comparison is made regarding the efficacy of these algorithms vis-à-vis other standard machine learning methods like simulated annealing, basin hopping, artificial bee colony and Bonobo algorithms.

Representative publications:

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