PREDICTION OF THE STRUCTURE AND STABILITY OF MOLECULES AND CLUSTERS

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The unique properties of nanoclusters are extensively used in nanoelectronics, optoelectronics, solar cells, catalysis, biomedical imaging sensors, etc. These properties are closely linked to the atomic structure of particles, especially in small clusters. In this work we present a new method for prediction of atomic structure and stability of nanoclusters in a wide area of sizes and compositions. Our algorithm performs joint evolutionary search for all clusters in a given area of the compositional space and takes advantage of common structural motifs often observed in clusters of close composition. The new algorithm was implemented in the widely used code USPEX [1].

We apply our method to global optimization of a number of systems, including Si-O [1], Cu-Au [2] and Li-P [3] nanoclusters in a wide range of compositions. Scanning over wide composition areas reveals trends in cluster structure and related properties. In particular, we calculated the minimum second derivative of energy with respect to the number of atoms of different types, which allows one to find so-called “magic” (especially stable) clusters, which can be interesting for different applications.

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References

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