

Department of Physics & Astronomy

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Friday, November 18, 2011

Time: 3:00 p.m. - 4:00 p.m.

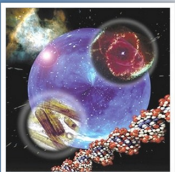
BB 3.04.18

Searching for the structures of nanoclusters and nanoalloys

The computational exploration of the energy landscape of nanoparticles is a very difficult task due to the enormous number of different possible geometric structures, corresponding to distinct local energy minima. In the case of bi- or multi-component systems, such as nanoalloys, the problem is even more difficult, because the structures can differ not only in geometry, but also in chemical ordering.

The problem of finding the lowest-energy structure for a given nanoparticle size and composition is known as "global optimization" problem.

Here, global optimization methods are reviewed, with emphasis on the basin-hopping method and its refinements. Applications to nanoalloys such as AgCu, CoPt and AgAu are presented.



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