Computational engineering of bimetallic nanocrystals with tailor-made atomic ordering

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Metal nanoparticles (NPs) are key component of numerous materials. Yet, monometallic NPs are often insufficiently versatile, which limits their use. Conversely, diversity of mixed-metal NPs (nanoalloys) enables tailoring their properties for a particular application much easier. However, the complexity of nanoalloys hinders the understanding of their structure-property relations. It is very laborious to experimentally determine the atomically resolved composition (atomic ordering) in nanoalloys. We recently developed an innovative method to predict atomic ordering in nanoalloys from results of density functional calculations [1]. This efficient method is applicable to various combinations of transition metals with each other and with *s*,*p*-elements [1-5]. It allows one to reliably predict the thermodynamically stable atomically resolved 3-dimensional structures of nanoalloys, thus guiding their manufacturing. The method also permits to assess structural changes in nanoalloys *i*) at elevated temperature, *ii*) under reaction atmosphere or *iii*) on a support. We shall outline the method and present examples of its application to a variety of nanoalloys based on Pd [1], Pt [2-4] and Ni [5].

Our new method renders possible generating databases of structures and energies of alloy NPs spanning the Periodic Table. Its applications will deepen the general understanding of chemical bonding in nanoalloys and radically accelerate the discovery of tailor-made nanoalloy materials. Simplicity and reliability of this approach provide unique opportunity for real-time simulating various kinds of nanoalloy particles with thousands of atoms.

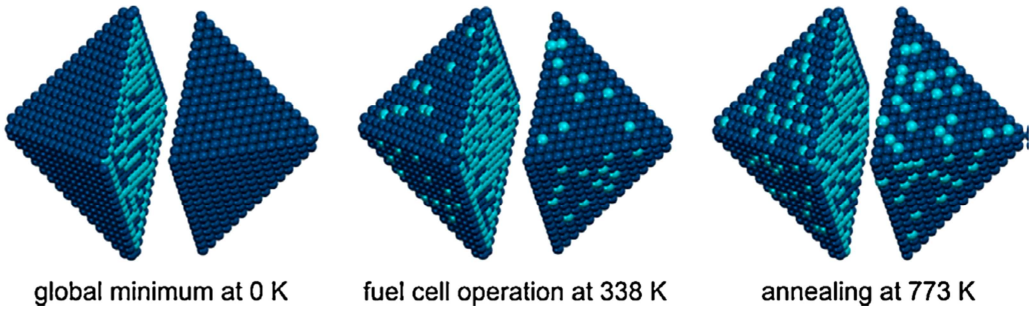

Figure 1: Temperature-dependent structures of $Pt_{1638}Co_{1637}$ particles [3]. Pt – dark blue.

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