Computational design of advanced nanoalloy materials for catalysis and beyond

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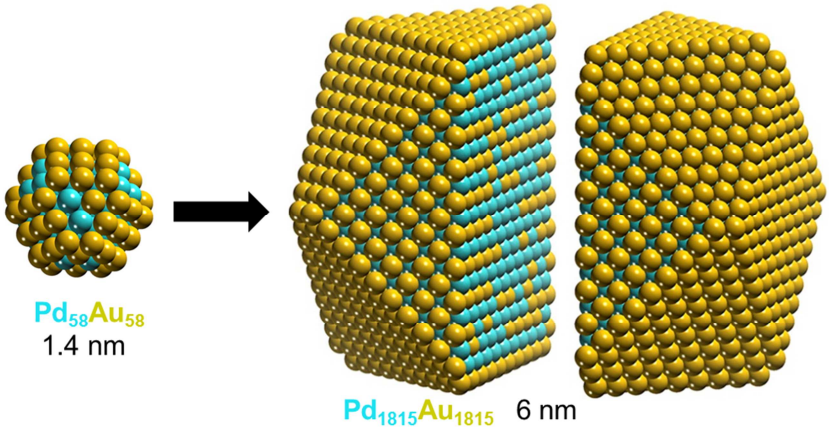
Metal particles are key components of many functional materials, including catalysts. Nevertheless, insufficiently versatile properties of monometallic particles limit their usage and mixed-metal particles (nanoalloys) often become systems of choice for a given application. However, it is very challenging to determine the atomically resolved structure (chemical ordering) of nanoalloys, which is required for rationalizing their reactivity and related properties. We developed a method [1,2] to optimize chemical ordering in nanoalloys of different metals using density-functional calculations. The method allows predicting energetically stable structures of crystalline nanoalloys with thousands of atoms, which can be then manufactured on the knowledge-driven basis.

I will outline the method and illustrate results of its applications to nanoalloys of Pd [1,2], Pt [3-5] and Ni [6] with *d*- and *s,p*-metals. A special case of bimetallic catalysts exposing surface sites composed of single atoms of an active metal surrounded by atoms of the second metal will be briefly addressed. Efficiency of our method opens an opportunity to systematically model nanoalloys of various metals spanning the Periodic Table. Applications of the method are able to accelerate design of tailor-made nanoalloys and deepen understanding of the bonding in nanoalloys.



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