New taxonomy of platinum nanoclusters

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The unexpected diversity of metallic nanoclusters' inner structure has now been catalogued into families. Physicists have gained new insights into the inner intricacies of the structural variations of metallic nanoclusters. This work by Luca Pavan, Cono Di Paola and Francesca Baletto from King's College London, UK, is about to be published in *European Physical Journal D*. It takes us one step closer to tailoring on-demand characteristics of metallic nanoparticles. Indeed, the geometric structure of these nanoclusters influences their chemical and physical properties, which differ from those of individual molecules and of bulk metals.

The problem resides in the difficulty in evaluating the optimal structure for such clusters in order to make them display specific properties and satisfy a particular technological need. This is because a system consisting of several interlinked atoms is far too complex for its optimal structure to be identified simply by resolving equations.

Instead, the authors applied a numerical simulation method, known as metadyamics, typically used to sample the energy landscape of biomolecules and proteins. This technique, quite new in the field of metallic nanoparticles, identifies structures corresponding to each minimum of the energy landscape. In addition, this approach gains a better insight into the interconnection of various structural motifs at given temperatures.

Specifically, this study describes an iterative approach for metadynamics in order to detect which are the key structures of 13-atom-strong

platinum nanoclusters. The authors focused on identifying the most recurrent motifs that can play an important role during structural transformations of the nanoclusters.

In addition, the team proposed a complete way of cataloguing such structural motifs in families. The next step would be to understand how different geometrical shapes are connected and evaluate the energy cost for each transformation, from one type of geometry to another. Applications could, for example, be found in nanocatalysis and nanodevices for magnetic storage.

More information: Pavan L., Di Paola C. and Baletto F. (2013), Sampling the Energy Landscape of Pt13 with Metadynamics, *European Physical Journal D*, DOI 0.1140/epjd/e2012-30560-y

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