Faculty of Chemistry and Pharmacy, Sofia University, Bulgaria

Horizon2020
Materials Networking

On **May 28**, 2019 at **16:00** h in the Conference Hall of FCP-SU

Prof. Konstantin Neyman

Faculty of Chemistry, University of Barcelona, Spain

will present a lecture on

In-silico design of bimetallic nanocrystals

Bimetallic particles (nanoalloys) often become systems of choice for various applications. However, determining atomic ordering in nanoalloys, which largely defines their properties, is very challenging. We developed a method to search for thermostable atomic orderings in nanoalloys by first-principles (DFT) calculations combined with a topological description [1,2]. The method allows to reliably predict energetically most stable in vacuum structures of bimetallic crystallites with up to thousands atoms and to estimate how their surface atomic ordering will be modified in a given reactive environment [3-5].

The talk will overview our recent results of application of this novel approach to nanoalloys of Pd [1,2,4,5], Pt [6-8] and Ni [3] with *d*- and *s,p*-metals. Usage of this method can radically accelerate design of tailor-made nanoalloys for broad variety of technological needs and deepen general understanding of the bonding in nanoalloys.

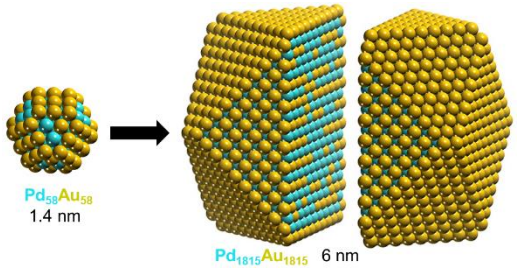

Figure. *Topological descriptors derived from DFT calculations of several dozen different atomic orderings of a bimetallic nanocrystallite open a way to predict atomic ordering in much larger nanoparticles not assessable for DFT treatment.*

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