Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular dynamics simulations of bimetallic nanocatalysts, guided by X-ray Absorption Fine Structure data[1] JANIS TIMOSENKO, ANATOLY FRENKEL, Stony Brook University — Small bimetallic nanoparticles (with sizes below 4 nm) are a promising material for various applications, e.g., in the field of catalysis, in particular, due to the possibility to tailor their properties by changing their size, shape, chemical composition and intra-particle distributions of both metals. To fully exploit these properties, it is necessary to gain a deep understanding of relation between these degrees of freedom and nanoparticle (NP) atomistic structure and dynamics. It was demonstrated during the last decade that theoretical simulations, such as molecular dynamics (MD) simulations, may be very helpful for this purpose. The structure models, obtained in MD simulations, however, need to be validated by experimental data. In this study we demonstrate that Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy can be successfully used for such validation, since it is a unique, chemically sensitive method that is able to provide detailed information on the distributions of atoms within NPs and on their dynamics. The potentiality of such combined MD-EXAFS approach is illustrated in this study on the example of bimetallic PdAu NPs, synthesized using peptide template method.

[1]We gratefully acknowledge support from the National Science Foundation under the DMREF program Grant No. CHE-1534184.

Janis Timosenko
Stony Brook University

Date submitted: 02 Nov 2016 Electronic form version 1.4