Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Atomistic simulations of activated processes in nanoparticles synthesis[1] FEDERICO GIBERTI, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — Core-shell and Janus nanopartices are promising building blocks for new, highly efficient solar cells. One of the most common synthetic pathways to produce such nanostructures is the use of cation exchange reactions. Although widely used, these procedures are not completely understood. We employed classical Molecular Dynamics and Monte Carlo simulations to understand these transformation at the molecular level; in particular we investigated the conversion from CdSe (sphalerite) to PbSe (rocksalt) NPs with 2-3 nm diameter. In order to recover the equilibrium free energy surfaces we used state of the art enhanced sampling techniques, including Metadynamics. The formation of hybrid core-shell structures resulted to be an activated process, where the limiting step is the transition of a sphalerite to a rocksalt PbSe nucleus. We found that the barrier height and the stability of the two phases depend on the size of the PbSe nucleus, suggesting that the process could proceed via a two step mechanism, where a small sphalerite nucleus is formed first, and it then transforms to a rocksalt nucleus. Our results give insight into possible manipulation processes at the molecular scale, which could be used to stabilize metastable NPs and tune their physical and chemical properties.

[1]This work was supported by the DOE grant No. DE-FG02-06ER46262

Giulia Galli
Institute for Molecular Engineering, The University of Chicago

Date submitted: 03 Nov 2015 Electronic form version 1.4