Understanding the Surface of CdSe Semiconductor Nanocrystals with Computational Chemistry

Ivan Infante

Faculty of Sciences, Department of Theoretical Chemistry, Vrije Universiteit Amsterdam, De Boelelaan 1083, 1081 HV, Amsterdam, The Netherlands
iinfant76@gmail.com

Colloidal semiconductor nanocrystals (NCs) are characterized by a large surface-to-volume ratio that renders them extremely sensible to processes occurring on the surface.[1] The capping ligands, used to stabilize the nanocrystal in an organic solvent, play an important role in influencing the structure and the optoelectronic properties of these materials.
Despite major progresses to characterize the chemical reactions occurring on the surface of CdSe NCs, there are still several key questions to be answered on the nature of the NC-ligand interactions and how trap states, which are deleterious for charge transport, are formed on the surface.[2]
A leap forward in solving the above issues is to analyze the surface using theoretical simulations. Based on a combination of Density Functional Theory and Molecular Dynamics simulations, we present the first multiscale modeling of real sized CdSe QDs (about 4.0 nm) capped with oleate ligands and immersed in an organic solvent like dichloromethane with a simulation box containing 25000 atoms.[3] Molecular dynamics simulations, carried out up to the microsecond timescale, provide crucial insights on the surface dynamics, and the role of the ligands on the structural optoelectronic properties of these materials.

References

[1] M.P. Hendricks, M.P. Campos, G.T. Cleveland, I. Jen-La Plante, J.S. Owen, Science, 340 (2016), 1226
[2] O. Voznyy, S.M. Thon, AH Ip, EH Sargent, J. Phys. Chem. Lett., 4 (2013), 987
[3] K. de Nolf, S. Cosseddu, I. Infante, Z. Hens, under review

Figures

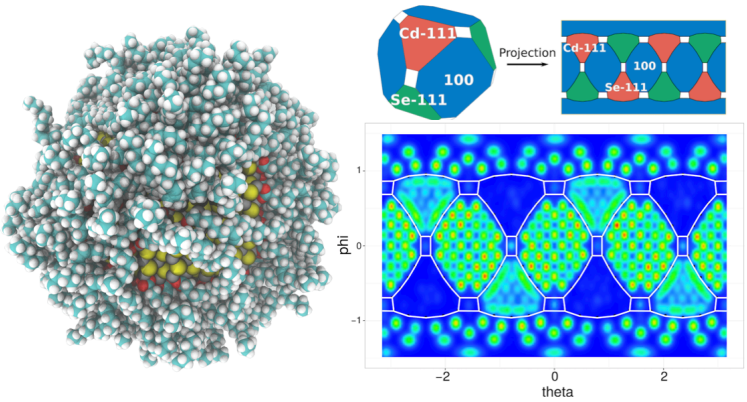

Figure 1: (left) Modelled CdSe NC; (right) Ligand distribution on the NC surface projected on a 2D plane.