An Automated Tool for the Construction of Semiconductor Nanocrystals

Juliette ZITO - *Istituto Italiano di Tecnologia*

The recent improvements in computer architectures nowadays allows for the atomistic simulation of large composite molecular systems and establishes computational chemistry as a powerful tool to describe colloidal semiconductor nanocrystals with increasingly realistic sizes and shapes.[1,2] For all such atomistic simulations, a recurring task is the generation of initial structures, consisting of Cartesian coordinates of all atoms in the system. Without these structures no calculation is possible, and, in many cases, this step forms a critical bottleneck in the workflow of designing and running the simulation on a supercomputer.[3,4] In this context, we present a Python-based package for the automated preparation of semiconductor nanocrystals models that can then be used directly either in quantum or classical chemistry simulations. The size, shape and faceting of such models are chosen by the user based on the experimental evidence available for that specific semiconductor nanocrystal and case study, thus allowing to obtain increasingly realistic atomistic models.