Atomistic modelling of quantum dots: core-shell and bismuth chalcohalide nanocrystals

Gabriele SALEH - *Istituto Italiano di Tecnologia*

The synthesis of semiconductors in form of colloidal nanoparticles, commonly known as quantum dots (QDs), have opened a wide range of new possibilities concerning their employment in optoelectronic devices. This is because the properties of nanocrystals are radically different from their bulk counterpart, and the quantum confinement associated with their nanodimension allows to tune the properties of the particles by changing their size, shape, and surface termination. These structural and electronic details are fundamental for the design of better performing QDs but, on the other hand, are difficult to be measured experimentally. Therefore, atomistic modelling plays a key role in this field.
Our group develops computational tools and protocols for the study of QDs in close collaboration with the experimental groups of our institute. In this contribution, two relevant examples of application will be discussed. The first is the core-shell InAs@ZnSe QDs. A newly developed synthetic route allowed to reach the record-high infrared quantum yield of 70%. We implemented a protocol to obtain a realistic atomistic model of these QDs. The structural features that allowed the growth of thick ZnSe shells will be presented, along with a discussion of the electronic structure which challenges the commonly adopted band alignment models adopted for these systems. The second example concerns bismuth chalcohalides, and in particular the compound $Bi_{13}S_{18}X_2$ (X=Br,I). Our density functional theory simulations resolved the crystallographic disorder and revealed the presence of subvalent Bismuth dimers Bi_2^{4+}. The electronic structure will be discussed in this contribution, demonstrating how the formation of these exotic chemical entities result from Peierls distortions.