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Tuning the structural and electronic properties of heterogeneous chalcogenide nanostructures[1] FEDERICO GIBERTI, Univ of Chicago, MARTON VOROS, Argonne National Laboratory, GIULIA GALLI, Univ of Chicago and Argonne National Laboratory — Heterogeneous nanostructures, such as quantum dots (QDs) embedded in solid matrices, are promising platforms for solar energy conversion. Unfortunately, there is scarce information on the structure of the interface between the dots and their embedding matrix, thus hampering the design of functional materials with desired optoelectronic properties. Here, we developed a hierarchical computational strategy to obtain realistic models of semiconductor QDs embedded in matrices using enhanced sampling classical molecular dynamics simulations and predicted their electronic structure using first-principles electronic structure methods. We investigated PbSe/CdSe systems which are promising materials for solar cell applications and found a favorable quasi-type-II band alignments both for PbSe QDs in CdSe matrices and for CdSe embedded in PbSe. However, in the former case, we found the presence of detrimental intra-gap states, while in the latter no defect states are present. Hence we predict that embedding CdSe in PbSe leads to a more efficient platform for solar energy conversion. In addition, we showed that the structure of CdSe QD and in turn its band gap might be tuned by applying pressure to the PbSe matrix, providing a way to engineer the properties of new functional materials.

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