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A theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core/shell nanoparticles MICHAEL SPRINGBORG, PRANAB SARKAR, University of Saarland, Saarbruecken, Germany, GOTTHARD SEIFERT, Technical University of Dresden, Germany — We present a theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core/shell nanoparticles. The results are relevant not only for understanding the properties of these nanoparticles but also for understanding those of quantum dots. We have considered nanoparticles whose structures were obtained as relaxed structures of essentially spherical parts of the zincblende crystal structure and with one semiconductor compound outside the other one. The electronic properties and the total energy for a given structure were calculated using a parameterized density-functional tight-binding method. The results give information on structure, electronic properties, the HOMO and LUMO orbitals, the charge distribution, and the stability of these core/shell nanoparticles. The results depend critically on the size of both core and shell, and only in one single case we find a charge separation upon excitation. We have also investigated the energetics related to the interchange of a S and a Se atoms between the core and the shell. Although the total energy may be lowered upon interchange, the energy barrier for this process is so large that the systems should be stable against degradation.

Michael Springborg
University of Saarland, Saarbruecken

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