Vibrational properties of II-VI semiconductor quantum dots

The phonon dispersion (the energy spectrum of vibrational modes) is an important property of all materials and has a strong effect on the optical properties. In a "0-dimensional" quantum dot the phonon bands known from 3-D bulk materials collapse into discrete vibrational modes. These modes, or vibrons, therefore differ from the bulk modes and depend on the size of the quantum dot and the material constituting them. In order to be able to predict these vibrational properties, we parametrize an effective model based on ab-initio calculations using density functional theory (DFT).

The Bachelor or Masters project consists of conducting ab-initio ground-state calculations for a range bulk II-VI semiconductors (CdS, CdSe, CdTe), starting with the zinc-blende phase, and thereby obtaining the parameters needed for these materials. The effect of quantum dot size and structure can then be examined directly. We have found that the phonon dispersion calculated in this way for III-V semiconductors are in very good agreement with considerably more expensive ab-initio calculations based upon the frozen-phonon method in DFT[1]. The interesting lead chalcogenides (PbS, PbSe, PbTe) can also be directly considered. After successfully considering the zinc-blende structure, the more complicated wurtzite structure can also be addressed. The long-term goals (beyond this Bachelor or Masters project) will be to use these potentials to study the impact of vibrations on the electronic and optical properties of quantum dots. Also the time evolution of excited states (how fast a hot quantum dot can cool down) will require the use of the derived potentials. The project will be a collaboration with Dr Peng Han (Captiol Normal University, Beijing).

References

[1] P Han and G Bester. Interatomic potentials for the vibrational properties of III-V semiconductor nanostructures. *Physical Review B*, 83:174304–1–8, 2011.