Efficient atomistic calculation of excitonic properties of crystal-phase quantum dots

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Excitonic properties of novel nanostructures such as crystal-phase quantum dots or semiconductor quantum wires are difficult to calculate with first-principle modelling such as the density functional theory (DFT) due to their size, often exceeding millions of atoms. On the other hand, simplified methods such as the effective mass approximation do not correctly account for all effects of symmetry, alloying, lattice randomness, interface effects or crystal phase symmetry.

Here we present results of the excitonic calculations of a multi-million atom InP crystal-phase quantum dot. To calculate the single-particle spectra, we used the empirical nearest-neighbor tight-binding model and the Lanczos algorithm for Hamiltonian matrix diagonalization. For many-body calculations, we used a novel real-space [1] approach, utilizing Fourier-space methods in order to achieve quasi-linear computational complexity with the respect to the number of atoms. We show that our linear scaling method gives results consistent with the traditional linear combinations of atomic orbitals (LCAO) approach, but at the same time, allows to model nanostructures containing $\sim 10^7$ atoms.

[1] P. T. Różański, M. Zieliński, *Phys. Rev. B* **94**, 045440 (2016).