Empirical tight-binding model for crystal phase quantum dots

M. Patera[1] **and M. Zieliński**[1]

[1] *Institute of Physics, Nicolaus Copernicus University, Grudziądzka 5, 87-100 Toruń, Poland*

Atomistic modelling of nanostructures composed of mixed crystal phases, such a wurtzite and zinc blende InP crystal phase quantum dots [1], presents a significant theoretical and computational challenge. In this work we present an empirical tight-binding [2] model with d-orbitals and spin-orbit interaction for zinc blende and wurtzite mixed systems that accounts for valence band-offsets between both phases, larger wurtzite band gap and crystal field splitting in wurtzite. We account for atomic d-orbitals splitting due to low lattice symmetry and utilize a generic fitting algorithm to obtain bulk parameter sets that accurately reproduced energies and effective masses in high-symmetry points. Finally we illustrate our model on the example of realistic size crystal phase quantum dots.

[1] M. Bouwes Bavinck, K. D. Jöns, M. Zieliński, G. Patriarche, J.-C. Harmand, N. Akopian, and V. Zwiller, *Nano Lett.* **16**, 1081 (2016).
[2] M. Zieliński, M. Korkusiński, and P. Hawrylak, *Phys. Rev. B* **81**, 085301 (2010).