Electric field effect on excitonic spectra of crystal phase quantum dots

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Zinc blende stacking faults in InP wurtzite nanowire can bind excitons and are known as crystal phase quantum dots [1]. In this work we study the effect of external electric field on excitonic spectra of such systems. From modeling point of view this is a formidable challenge since crystal phase quantum dots are multi-million atom type-II nanostructures. In such structures holes are delocalized over a nanowire of mesoscopic dimensions, whereas electrons are confined in nanoscale, few-monolayer-thick regions. We compare several approaches of electric field treatment: exact diagonalization, self-consistent tight-binding calculation and hybrid methods. Finally, we propose a multi-configurational self-consistent approach, originally developed to efficiently and accurately treat similar problems. This approach is not limited to crystal phase quantum dots, but may also find applications in atomistic modeling of other nanostructures, such as transition metal dichalcogenide layers or phosphorous multi-dopant problems in silicon.

[1] M. Bouwes Bavinck, K. D. Jöns, M. Zieliński, G. Patriarche, J.-C. Harmand, N. Akopian, and V. Zwiller, *Nano Lett.* **16**, 1081 (2016).