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Excitonic absorption of million-atom (In,Ga)As/GaAs self-assembled quantum dots[1] GUSTAVO A. NARVAEZ, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401 — We calculate the optical absorption spectra of (In,Ga)As/GaAs self-assembled quantum dots by adopting an atomistic pseudopotential approach to calculate the single-particle electron and hole confined states of the dot followed by a calculation of the neutral exciton X^0 states $|\Psi^{(\nu)}(X^0)\rangle$ based on the configuration-interaction approach. We predict three types of *allowed* transitions that would be naively expected to be forbidden. (i) Transitions involving low-lying electron and hole states that are forbidden in simple effective mass models (e.g. $1S$-$2S$, $1S$-$1P$) become allowed by virtue of single-particle band-mixing. (ii) Transitions involving a deep hole state, with a mixture of heavy-hole and light-hole character, and an electron in the lowest state are found to have oscillator strengths that are comparable in magnitude to those of the expected allowed transitions. Thus, simple models based on single-band envelope functions cannot predict these transitions. (iii) Transitions whose intensity is large due to many-body borrowing of oscillator strength from allowed transitions. The transitions in (i) and (ii) appear, respectively, as low-energy and high-energy satellites of the allowed P-P transitions, as observed in PLE.

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Gustavo A. Narvaez
National Renewable Energy Laboratory, Golden, Colorado 80401

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