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Shape, charge, and alloy fluctuation effects on optical properties of million-atom InGaAs/GaAs dots[*] GUSTAVO A. NARVAEZ, GABRIEL BESTER, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401 — Single-dot spectroscopy makes it possible to probe in detail dot-to-dot changes in optical properties of self-assembled $In_{1-x}Ga_xAs/GaAs$ dots. An atomistic pseudopotential method combined with the configuration interaction approach reveal the role of shape, charge, and alloy fluctuations on the electronic structure, polarization of optical transitions, and excitonic radiative lifetimes of $In_{0.6}Ga_{0.4}As/GaAs$ quantum dots. Several features emerge. (i) *Height fluctuations.* Recombination energies and excitonic binding of X^0 (neutral exciton), X^-, X^+, and XX (biexciton) change significantly with height, but not with randomness. (ii) *Charge fluctuations.* The lowest transitions of X^- and X^+ are naturally unpolarized, whereas those of X^0 and XX are polarized in plane. Thus, charge fluctuations affect polarization of an ensemble of dots. (iii) *Alloy fluctuations.* Different random realizations (configurations) of the same alloy dot lead to radically different polarizations of transitions in X^0 and XX. In the light of our simulations, we discuss dramatic changes in polarization recently observed in InAs/GaAs single dots.
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