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Theory of InP nanocrystals under pressure J.G. DIAZ, G.W. BRYANT, W. JASKOLSKI, National Institute of Standards and Technology, Gaithersburg, MD 20899-8423 — An empirical tight-binding theory which includes the effects of the relaxation of the lattice is employed to investigate the role of an external hydrostatic pressure on the opto-electronic properties of InP nanocrystals. For the bulk, our model describes accurately the evolution of the lowest conduction band-edges with pressure and predicts the Γ_{1c}-X_{1c} crossover at the same lattice contraction as measured in the experiment. For small InP nanocrystals, the bandgap dependence on pressure predicted with this model is, for the first time, in agreement with the experimental results. Previous atomistic models, which assumed a bulk-like arrangement for the atoms in the nanocrystal under pressure, led to negligible mixing of the Γ_{1c}- and L_{1c}- minima and did not account for the increasing localized character of the electron and hole states as a function of pressure. The lattice-relaxed tight-binding model suggests a mechanism for the experimental red-shift different from the Γ_{1c}-X_{1c} crossover predicted by bond-distance scaling models. In the lattice-relaxed model, the experimental red-shift is explained as a transition from bound states localized inside the dot to surface-like states in the dot exterior. The evolution of the near-band-edge optical spectra as a function of pressure has been analyzed for different nanocrystal sizes, geometries and degrees of surface passivation with both the bond-length scaling and lattice-relaxed tight-binding approaches.

Jose Gabriel Diaz Garcia
NIST, Gaithersburg, MD 20899-8423

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