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Quantum-size-induced phase transitions in quantum dots: Indirect-band gap GaAs nanostructures ALEX ZUNGER, JUN-WEI LUO, ALBERTO FRANCESCHETTI, National Renewable Energy Lab — Quantum nanostructures are often advertised as having stronger absorption than the bulk material from which they are made, to the potential benefit of nanotechnology. However, nanostructures made of direct gap materials such as GaAs can convert to indirect-gap, weakly-aborbing systems when the quantum size becomes small. This is the case for spherical GaAs dots of radius 15 Å or less (about 1000 atoms) embedded in a wide-gap matrix. The nature of the transition: Γ-to-X or Γ-to-L is however, controversial. The distinction can not be made on the basis of electronic structure techniques that misrepresent the magnitude of the various competing effective mass tensors (e.g, LDA or GGA) or wavefunction coupling (e.g, tight-binding). Using a carefully fit screened pseudopotential method we show that the transition occurs from Γ to X, and, more importantly, that the transition involves a finite V (Γ-X) interband coupling, manifested as an "anti-crossing" between the confined electron states of GaAs as the dot size crosses 15 Å. The physics of this reciprocal-space Γ-X transition, as well as the real-space (type II) transition in GaAs/AlGaAs will be briefly discussed.

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