

Abstract Submitted  
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**Electronic and optical fine structure of GaAs nanocrystals: the role of d orbitals in a tight-binding approach** J.G. DIAZ, GARNETT W. BRYANT, National Institute of Standards and Technology — Electronic structure and optical spectra of GaAs nanocrystals for a wide range of sizes are studied by using both  $sp^3s^*$  and  $sp^3s^*d^5$  nearest-neighbor tight-binding models. Our results show that the inclusion of  $d$  orbitals into a minimal basis set is necessary for a proper description of the lowest electron states, especially in the strong confinement regime. For dot sizes below 2.5 nm, the ground electron state is primarily built of L-point bulk band-states, giving the nanocrystals indirect-gap character. Simpler  $sp^3s^*$  models yield an incorrect description of electron states made from bulk band-states away from the Brillouin zone center. In contrast,  $sp^3s^*d^5$  models are able to provide a consistent picture of the main optical features in agreement with experiments.

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