

Abstract Submitted
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Jahn-Teller distortion in semiconductor nanocrystals¹ GUSTAVO M. DALPIAN, ALINE L. SCHOENHALZ, JEVERSON T. ARANTES, Universidade Federal do ABC — Semiconductor nanocrystals or quantum dots can present properties that are very different from their bulk counterparts. Quantum confinement and surface effects play important roles in determining these unusual properties. Here we report a Jahn-Teller distortion in pristine nanocrystals upon the addition of charges. Results will be presented for Si, InAs and CdSe nanocrystals. In order to observe this effect, we have performed calculations using the Density Functional Theory and hybrid functionals. We will discuss the implications of this distortion on the electronic and optical properties of these materials.

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Gustavo M. Dalpian
Universidade Federal do ABC

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