

Abstract Submitted
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Size and shape dependence of electronic and optical excitations in TiO₂ nanocrystals¹ KOPINJOL BAISHYA, SERDAR OGUT, University of Illinois at Chicago — We present results for the electronic structures, quasi-particle gaps, and the absorption spectra of TiO₂ nanocrystals of both rutile and anatase phases with various shapes, sizes, and surfaces exposed. We study the size and shape dependences of these electronic and optical properties, computed both within time-dependent density functional theory and many-body perturbation methods such as the GW-BSE, using appropriately passivated nanocrystals to mimic bulk termination. Surface effects are examined by using nanocrystals of various sizes with particular surfaces, such as (110) in rutile and (101) in anatase phases, exposed. We interpret the resulting optical absorption spectra of these nanocrystals in terms of the bulk spectra and compare them with predictions from classical Mie-Gans theory.

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