

Conical Intersections and Non-Radiative Recombination in Semiconductor Nanocrystals

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Non-radiative recombination limits the efficiency of semiconductor-based optoelectronic devices such as photovoltaic cells, photocatalysts, and light emitting diodes by converting useful electronic energy into heat. It has been known for more than half a century that such recombination is facilitated by defects, but theoretical prediction of exactly which defects promote non-radiative recombination remains a challenge. In order to develop a predictive understanding of the role specific defects play in semiconductor photophysics, we are investigating the hypothesis that conical intersections introduced by defects form pathways for recombination. The accurate identification of such intersections is computationally challenging, thus we have developed new multireference electronic structure and molecular dynamics methods and graphics processing unit accelerated software for this purpose. Identification and characterization of such intersections elucidates the effects of oxidation and other postsynthetic modifications on the photoluminescence spectrum of nanostructured silicon.