Electronic relaxation in graphene quantum dots: the role of non-adiabatic and spin-orbit coupling

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Quantum dots have received considerable attention as potential materials for photovoltaics because of their large electronic energy spacing due to quantum confinement. Recent experiment has demonstrated slow cooling in colloidal graphene quantum dots (GQDs) on time scales of 100-1000 ps (Mueller et al 2011, *Nano Lett,* 11, 56-60). However, the particular relaxation pathways that lead to these slow relaxation times are not well understood. Here, we investigate electronic relaxation in GQDs by modeling multiple relaxation mechanisms, including phonon-mediated non-adiabatic coupling and spin-orbit coupling, using first-principles calculations. Relaxation rates are then compared for GQDs in a colloidal environment to those embedded in a boron nitride matrix. Results from this investigation shed light on the crucial pathways limiting carrier relaxation and provide insight into the role of environment in relaxation rates. These findings will provide guidance in tailoring devices such as photovoltaics to maximize efficiency. Acknowledgment: This work is supported by DOE/BES DE-FG02-02ER45995.