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Biexciton-exciton cascades in graphene quantum dots

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Graphene quantum dots (GQDs) with engineered lateral size, shape, and edge allow for the modification of the electronic, optical and magnetic properties of graphene [1-5]. Here we present a theory of optical properties of GQDs [2-5]. Building on our previous work [1-4] we expand the single-particle wave functions in Pz carbon orbitals and compute energy spectra using the tight-binding model. The two-body Coulomb matrix elements are computed using Slater Pz orbitals, and screening is included through effective dielectric constant. The tight-binding calculation of single-particle states is followed by a fully self-consistent Hartree-Fock treatment of electron-electron interactions. We find a semiconducting state originating from the semi-metallic ground state of bulk graphene, followed by a Mott-insulating state with decreased screening. The semiconducting ground and excited state HF wave functions and energies are improved by inclusion of a limited number of multi-pair excitations using tb+HF+CI technique. We compute the evolution of the singlet and triplet exciton spectrum (G0W0-BSE) with size for different shape and edge type of quantum dots and compare with predictions based on confined Dirac Fermions[2].
The single exciton spectrum is compared with spectrum of exciton interacting with additional electron-hole pair excitations potentially leading to excitonic instability. We next move to exploit valley degeneracy and effects of additional layers. We focus on triangular colloidal graphene quantum dots [4,5] with the degenerate CB and VB band-edge and explore the possibility of creating coherent photon pairs in biexciton-exciton cascades. The spin-resolved bi-exciton spectrum, its Auger coupling and bi-exciton-exciton recombination spectrum are predicted and compared with measured optical properties of colloidal graphene quantum dots [4,5]. The theory of optical properties is extended to bi-layer graphene quantum dots.

[1]Guclu et. al., 2009 Phys. Rev. Lett. 103 246805
[2]Guclu et. al., 2010 Phys. Rev. B 82 155445
[3]Guclu et. al., 2013 Phys. Rev. B 87 035425
[4]Ozfidan et. al., 2014 Phys. Rev. B 89 085310
[5]Mueller et. al., 2010 Nano Letters 10 2679; Yan et. al., 2012 Acct. Chem. Research, DOI : 10.1021/ar300137p

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