Beyond graphene- Dirac Fermions in graphene quantum dots

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One can modify the electronic, optical and magnetic properties of graphene by engineering lateral size, shape, edge, number of layers and sublattice symmetry [1] in graphene quantum dots(GQD). Graphene quantum dots confine Dirac Fermions, both electrons and holes, with strength of their interaction controlled by both background dielectric constant and lateral confinement. Here we present new results describing the role of interactions in multi-exciton complexes composed of Dirac fermions in conduction and valence band, including theory of bi-excitons in small colloidal graphene quantum dots (GQD)[2,3,6] with a well-defined structure. The theoretical results are compared with transient absorption experiments [3]. Building on our previous work [1,5] we describe the single-particle energy spectra using the tight-binding model based on P_z carbon orbitals. All direct and exchange two-body Coulomb matrix elements are computed using Slater P_z orbitals for on-site and nearest and next nearest neighbors and approximated for farther neighbors. The Coulomb interactions are screened by a dielectric constant of external medium and sigma electrons changing the ratio of Coulomb interactions to the tunneling matrix element. For a given GQD with a defined shape, size, edge, and dielectric constant we compute the tight-binding single-particle states followed by a fully self-consistent Hartree-Fock calculation. The HF phase diagram of the GQD ground state as a function of the screened interaction strength is established. The many body ground and excited states are expanded in a finite number of electron-hole pair excitations from the Hartree-Fock ground state and computed using exact diagonalization technique with Hilbert spaces of the order of 10^6 configurations. This allows us to establish exciton and biexciton spectra and their Auger coupling[6]. For colloidal GQDs the degeneracy of the top of the valence and bottom of conduction band leads to characteristic X and XX bands shown in Fig.1. The transient absorption experiments probe this band and help us to identify possible XX-X-GS cascade as shown in Fig.1.

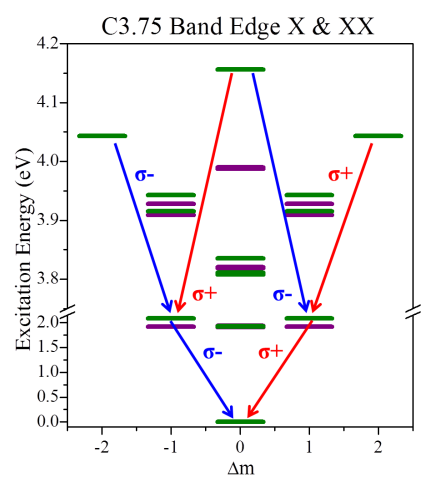

Fig.1 Bands of biexcitons and excitons in graphene quantum dots . XX-X cascade is indicated with red and blue arrows.

References

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