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Electron-electron and finite state interactions in optical properties of colloidal graphene quantum dots

Isil Ozfidan[1,2], Marek Korkusinski[1], Alev Devrim Guclu[1,3], and Pawel Hawrylak[1,2]

[1] *Quantum Theory Group, Security and Disruptive Technologies, National Research Council of Canada, Ottawa, Canada*
[2] *Physics Department, University of Ottawa, Ottawa, Canada*
[3] *Department of Physics, Izmir Institute of Technology, IZTECH, TR35430, Izmir, Turkey*

The electronic, optical and magnetic properties of graphene can be modified by engineering lateral size, shape, and edge [1-4]. Here we present new results describing the role of electron-electron and final state interactions in the optical properties of small colloidal graphene quantum dots (GQD)[1] with a well-defined structure, shown in Fig.1. Building on our previous work [2-4] we describe the single-particle energy spectra of P_z carbon orbitals using the tight-binding model. 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. All Coulomb matrix elements are screened by a dielectric constant of external medium controlling the ratio of Coulomb interactions to the tunneling matrix element. For a given GQD with a defined shape, size, edge, and dielectric constant we start with the tight-binding calculation of single-particle states followed by a fully self-consistent Hartree-Fock treatment. We construct a HF phase diagram of the GQD as a function of the interaction strength V relative to the tunneling matrix element t.

We find a semiconducting state originating from the semi-metallic ground state of bulk graphene, followed by a Mott-insulating state with decreasing screening. The ground state wavefunction and energy is improved by inclusion of a limited number of pair excitations using CI+Lanczos technique. For a semiconducting GQD ground state the singlet and triplet optical spectra, shown in Fig.1, are obtained by creating quasi-electron-hole pair excitations from the HF state and solving the Bethe-Salpeter equation. The bandgap renormalization and excitonic effects are analyzed as a function of GQD size, shape, and edge and compared with experiments on colloidal graphene quantum dots [1].

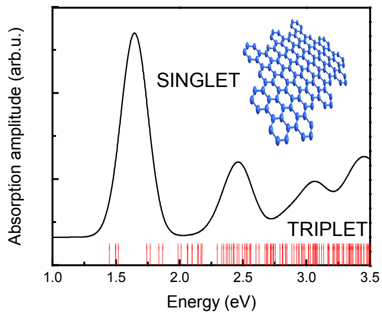

Fig. 1. Singlet and triplet exciton and absorption spectrum of a graphene quantum dot. Inset shows a schematic picture of the dot used in the calculation.

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