Abstract Submitted
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Theory of Two-Photon Absorptions in Graphene Fragments[1] K. ARYANPOUR, Dept of Physics, Univ of Arizona, A. SHUKLA, Dept of Physics, IIT Bombay, S. MAZUMDAR, Dept of Physics, Univ of Arizona, A. SANDHU, Dept of Physics and OSC, Univ of Arizona, A. ROBERTS, OSC, Univ of Arizona — Electron-electron correlations in graphene is currently an active field of research [1-3]. The carbon atoms in graphene have the same sp^2 hybridization as in strongly correlated π-conjugated polymer systems. The low energy behavior in graphene however appears to be reasonably described within the one-electron Dirac massless fermions model. Historically, the occurrence of the lowest two-photon state *below* the optical one-photon state provided the strongest proof for strong electron correlations in linear polyenes [4]. We systematically study the Coulomb interaction effects on the ground state and nonlinear absorptions in graphene fragments as a function of system size, beginning from the smallest stable fragment coronene. We report high order calculations of one- vs two-photon spin singlet and triplet states, in coronene, hexabenzocoronene and other molecular fragments that clearly indicate the strong role of electron-electron interactions. We will discuss the implications of our work on molecular systems for the thermodynamic limit of graphene.

[1] Siegel David A.; et al., PNAS, v108, 28, 11365-11369 (2011)
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[3] Uchoa B.; et al., arXiv: 1109.1577v1
[4] Ramasesha S.; et al., J. Chem. Phys. 80, 3278 (1984)

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