Abstract Submitted
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Evidence for strong electron correlations in graphene molecular fragments: Theory and experiments on two-photon absorptions[1] KARAN ARYANPOUR, Department of Physics, University of Arizona, ADAM ROBERTS, U.S. Army AMRDEC, Redstone Arsenal AL , ARVINDER SANDHU, Department of Physics and Optical Sciences Center, University of Arizona, ALOK SHUKLA, Department of Physics, IIT Bombay, India, SUMIT MAZUMDAR, Department of Physics and Optical Sciences Center, University of Arizona — Historically, the occurrence of the lowest two-photon state below the optical one-photon state in linear polyenes, polyacetylenes and polydiacetylenes provided the strongest evidence for strong electron correlations in these linear π-conjugated systems. We demonstrate similar behavior in several molecular fragments of graphene with D_{6h} symmetry, theoretically and experimentally. Theoretically, we have calculated one versus two-photon absorptions in coronene, two different hexabenzocoronenes and circumcoronene, within the Pariser-Parr-Pople π-electron Hamiltonian using high order configuration interaction. Experimentally, we have performed z-scan measurements using a white light super-continuum source on coronene and hexa-peri-hexabenzocoronene to determine frequency-dependent two-photon absorption coefficients, for comparison to the ground state absorptions. Excellent agreement between experiment and theory in our work gives strong evidence for significant electron correlations between the π-electrons in the graphene molecular fragments. We particularly benchmark high order electron-hole excitations in graphene fragments as a key element behind the agreement between theory and experiment in this work.

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