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The Electronic and Vibrational Properties of Carbon Nanorings
HANG CHEN, ANNA SWAN, Electrical and Computer Engineering Department and Photonics Center, Boston University — [n]-Cycloparaphenylenes ([n]-CPPs), carbon nanorings with n benzene units reminiscent of a single unit of a (n, n) armchair carbon nanotubes, show unusual optical behaviors: the absorption maximum is almost size independent at 340 nm, while the lower energy fluorescence exhibits multiple peaks with strong size dependence, opposite of quantum confinement behavior [1]. The energy levels for CPPs with various sizes are calculated using time-dependent density functional theory (TDDFT) and compared to the experimental results. Moreover, we calculate the Raman modes of various [n]-CPPs and propose that the multiple peaks observed in the fluorescence spectra could be due to the electron-phonon coupling effects. We also consider possible excitonic effects in these carbon nanorings, and discuss their similarities as well as differences to carbon nanotubes. [1] T. Iwamoto, Y. Watanabe, Y. Sakamoto, T. Suzuki, S. Yamago. *J. Am. Chem. Soc.*, 133, 2011;

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