Abstract Submitted
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First-principles studies of the optical properties of carbon nanohoops[1] JOYDEEP BHATTACHARJEE, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory — First proposed 70 years ago, cycloparaphenylenes – cyclic aromatic molecules that are the shortest possible segment of an armchair nanotube – have been only recently synthesized [1]. Using first-principles density functional theory and a Bethe-Salpter equation approach, we study structural, electronic, and optical properties of this novel class of materials, coined "carbon nanohoops." Remarkably, we find, in agreement with experiments, that smaller hoops have smaller optical absorption gaps. This counterintuitive trend, opposite to that expected from ordinary quantum confinement, reflects a large increase in electron-hole interaction strength with decreasing hoop diameter. The diameter dependence of this interaction is thoroughly explored for several nanohoops, compared with an acyclic series, and discussed in the context of possible applications. [1] R. Jasti, J. Bhattacharjee, J. B. Neaton, and C. R.Bertozzi, submitted (2008).

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