

Abstract Submitted
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Optical Excitations in Cycloparaphenylene Molecules of Various Sizes LYUDMYLA ADAMSKA, Theoretical Division T-1 and Center for Nonlinear Studies, Los Alamos Natl Lab, IFFAT NAYYAR, Center for Integrated Nanotechnologies (CINT), Los Alamos Natl Lab, ANNA SWAN, Department of Electrical and Computer Engineering, and Photonics Center, Boston University, STEVEN DOORN, SERGEI TRETIAK, Center for Integrated Nanotechnologies (CINT), Los Alamos Natl Lab — Cycloparaphenylene ($[n]$ CPP) molecule can be imagined as n benzene molecules connected in a periodic chain. $[n]$ CPPs with even number of links have alternating dihedral angles of ± 34 degrees, whereas odd-numbered $[n]$ CPPs cannot adopt such a high symmetry configuration, so they have a “defect”: one of the rings is connected to its neighbors by dihedral angles of about 20 degrees. This “defect” plays a role of a localization site for an exciton. In this work we show that in $[n]$ CPPs with $n > 8$ the exciton is localized on 5-6 rings, which strongly reduce their dihedral angles, while preserving the ground state geometry on the rest of the rings. This occurs both in odd-numbered and, surprisingly, in even-numbered $[n]$ CPPs. We use electronic structure theory to address the spatial extent/properties of electronic wavefunctions and resulting electronic functionalities in $[n]$ CPP molecular chromophores. Localization of excitonic states due to electron-phonon coupling in cycloparaphenylenes invalidates Condon approximation and breaks optical selection rules, making these materials to be efficient emitters. The effect of solvent is also discussed.

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