Computational Study of Nonlinear Optical Properties of Carbon-Based Molecular Systems

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ABSTRACT

Nonlinear optical (NLO) materials are important for applications in photonics and optoelectronics. In this study, the effects of Li_3O, Na_3O, and K_3O superalkali doping on [6]cycloparaphenylene ([6]CPP) and methylene-bridged [6]CPP nanohoops were investigated using computational methods. The results show that superalkali doping improves the electronic and optical properties of the nanohoops, including reducing the HOMO–LUMO gap and extending light absorption into the visible and near-infrared regions. Among the studied systems, Li_3O@MB[6]CPP showed the strongest nonlinear optical response, with a first hyperpolarizability of 1.62×10^5au. These findings indicate that superalkali-doped carbon nanohoops have potential for advanced optical and optoelectronic applications.