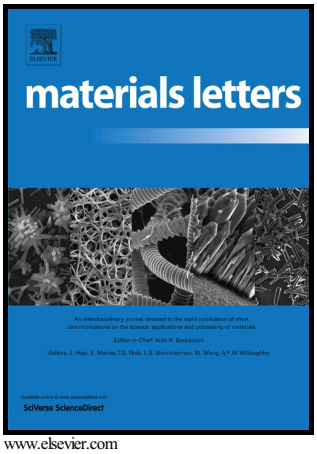

Computational determination of the Electronic and Nonlinear Optical properties of the molecules 2-(4-aminophenyl) Quinoline, 4-(4-aminophenyl) Quinoline, Anthracene, Anthraquinone and Phenanthrene

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Abstract

*The Electronic and Nonlinear Optical properties of the donor-acceptor molecules 2-(4-aminophenyl) Quinoline, 4-(4-aminophenyl) Quinoline, Anthraquinone; and the molecules Anthracene and Phenanthrene have been determined and some of these properties compared with literature values. The theoretical calculations were performed at the RHF level of theory and with two different hybrid density functional theories (DFT) (B3LYP and B3PW91), using the 6-31+G** basis set. The results show that these molecular systems have large average polarizability, anisotropy and first molecular hyperpolarizabilities. The small values of ε, and LUMO-HOMO energy band gap (E_{gap}) and the high values χ, η, <α>, and (β_{mol}) show that the molecules have very good electronic, nonlinear optical, optoelectronic and photonic applications. Furthermore, the (E_{gap}) of Phenanthrene shows that Phenanthrene is a good promising organic superconductor material.*

Keywords: Ab initio calculation, Semiconductors, optical materials, Superconductor, optoelectronics, photonics.