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Non-linear optical and electronic properties of oxa[n]circulenes: A theoretical insight

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In the current work, we have investigated the charge transport and Non-Linear Optical (NLO) characteristics of oxa[n]circulenes. Density functional theory (DFT) and Time dependent density functional theory (TD-DFT) are used to examine optoelectronic and NLO characteristics. TD-DFT calculations are utilized to simulate the absorption energies. Ionization potential (I.P.), electron affinity (E.A.), the frontier molecular orbitals (FMOs) i.e., Highest occupied molecular orbital (HOMO), Lowest unoccupied molecular orbital (LUMO) and HOMO-LUMO gap (E_{ge}) are calculated for the reported molecules. Nuclear independent chemical shift (NICS) values are generated to find aromatic behavior and stability of oxa[n]circulenes. Along with first and second hyperpolarizabilities, optoelectronic properties are also reported for the designed compounds.

Keywords: Oxa[n]circulenes, DFT, TD-DFT, Hyperpolarizabilities, NICS