From Halogenated Anthracenes to Bendable Displays: Decoding the Structure-Optical Gap Correlation

**Abstract**

In a world where electronics are a fundamental part of everyday life, bendable displays with tunable optical gaps are the future of this sector. To determine the validity that halogenated anthracenes and linear aromatic hydrocarbons in general have on the future of this industry, high level quantum mechanical computations were deployed on hundreds of structures of substituted benzene, naphthalene, and anthracene. An in-depth analysis of each halogenated structure shows that the energies of molecular orbitals, specifically the width of the optical gap, is a function of halogens’ size, electronegativity, and position on each aromatic ring within a molecule. Interestingly, the lowest optical gap has been found for a structure with the largest molecular polarizability.