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Quantum mechanical calculations in prediction of properties of π-conjugateded molecules

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The relevance of studies on π-conjugated molecular systems is determined by their wide application in modern organic electronics, photonics, sensing, and biomedical technologies. Quantum-mechanical calculations make it possible to predict the geometric, electronic, and spectral properties of π-conjugated molecules and their complexes with nanostructures at the stage of material design. This enables purposeful modification of molecular structures and control of the energy gap, charge transfer, and optical characteristics, which is important for the development of efficient organic semiconductors, photosensitive materials, nanocomposites, and bioactive systems.

Quantum-chemical calculations and spectral studies of π-conjugated molecules have revealed the features of the formation of their electronic structure and geometry. It has been shown that neutral 1,2-squaraines exhibit a polyene type of conjugation with pronounced bond-length alternation and a large energy gap, whereas isomeric 1,3-thiasquaraines demonstrate a polymethine type with nearly equalized bond lengths and a smaller energy gap. The introduction of heteroatoms and modification of donor–acceptor terminal groups significantly affect the geometry of the conjugated chain and the HOMO–LUMO gap. Charge injection into one-dimensional π-systems leads to the formation of soliton-like waves of charge and bond-length alternation and to the appearance of additional electronic states within the band gap. Studies of thin films of squaraine and merocyanine dyes have shown that intermolecular interactions between conjugated systems result in aggregates with different geometries, manifested as bathochromic or hypsochromic shifts of the absorption maxima.

It has been shown that the interaction of π-conjugated molecules with carbon nanostructures significantly modifies their electronic properties. In complexes of dyes with fullerene C60, graphene, and carbon nanotubes, charge transfer from the dye to the nanostructure occurs, accompanied by changes in bond lengths, shifts of electronic levels, and a reduction of the energy gap. Functionalization of fullerenes with covalent bridges or metal atoms breaks the symmetry of the C60 molecule, leading to the splitting of degenerate electronic levels and modification of vibrational spectra. Studies of metal doping and diffusion in C60 fullerite films revealed the possibility of forming dimeric and polymerized structures, accompanied by changes in X-ray diffraction patterns, vibrational spectra, and photoluminescence, and also demonstrated the possibility of complex formation between fullerenes and biologically active molecules.

The obtained results demonstrate that quantum-mechanical calculations are an effective tool for predicting the geometric, electronic, and spectral properties of π-conjugated molecules and their complexes with nanostructures. The revealed relationships between molecular structure, intermolecular interactions, and charge transfer can be used for the targeted design of new functional materials for organic electronics, photonics, and biomedical applications.

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