

delocalization

Redistribution of the valence-shell *electron density* throughout a molecular entity as compared with some localized models (individual atoms in their valence states, separated bonds or fragments). Different topological modes of the electron delocalization include:

(a) ribbon delocalization of either π - or σ electrons (*i.e.*, electrons occupying respectively π - and σ -orbitals); (b) surface delocalization of σ -electrons occurring through an overlap of radially oriented σ -orbitals of a cyclic molecule, as is the case of cyclopropane; and (c) volume delocalization of σ -electrons through an overlap of σ -orbitals directed inside a molecular polyhedron, as is the case in tetrahedrane.

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N.B. This supersedes an *earlier definition*.