

A04-6

Theory and quantum design for open-shell and three-dimensional aromatic characters induced in closely-stacked antiaromatic molecular systems

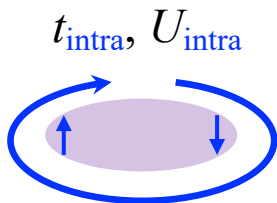
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Our Mission: Beyond condensed conjugation

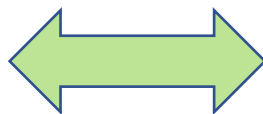
Aims of A04-6

- Establishing theory for intra-/inter-molecular (de)localization in closely-stacked antiaromatic molecular systems
- Extracting structure-property relationship and constructing design guidelines based on open-shell and aromatic characters

Open-shell and aromatic characters in monomer

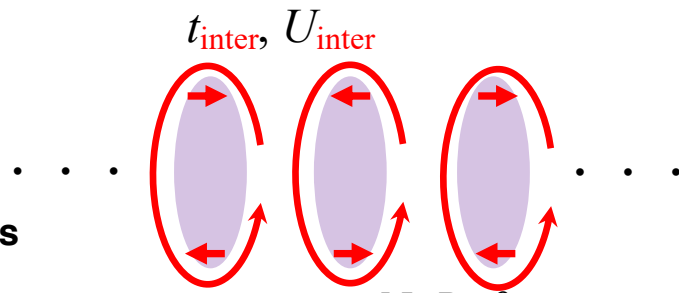


Effective physical model



Quantum chemical analysis

Open-shell and aromatic characters in aggregates



N, R, θ, \dots

Quantum design of
intramolecular delocalization

Quantum design of
intermolecular delocalization