

A04-6

Effective modeling condensed conjugation and exploration of charge-spin coupled phenomena

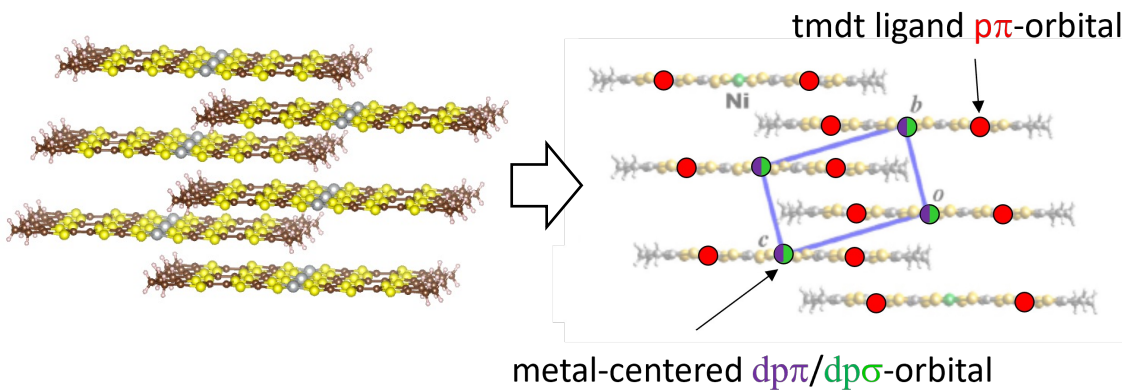
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Our Mission: Beyond condensed conjugation

Our aim in A04-6

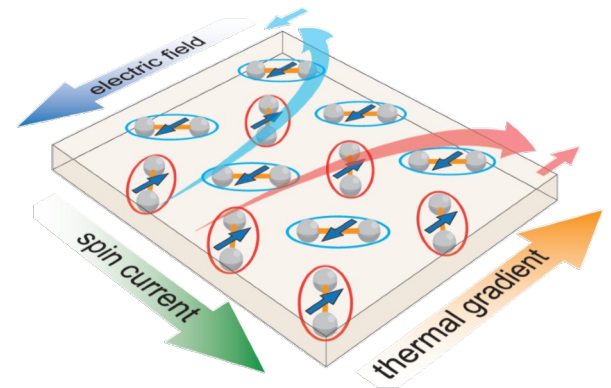
- Constructing quantitative effective models for condensed conjugation materials using ab initio first-principles calculations
- Theoretical exploration of novel electromagnetic response

Effective models for metal-containing molecular conductors



extracting intramolecular degree of freedom
& model analysis

novel spin transport properties



combination of molecular arrangement
and magnetic order