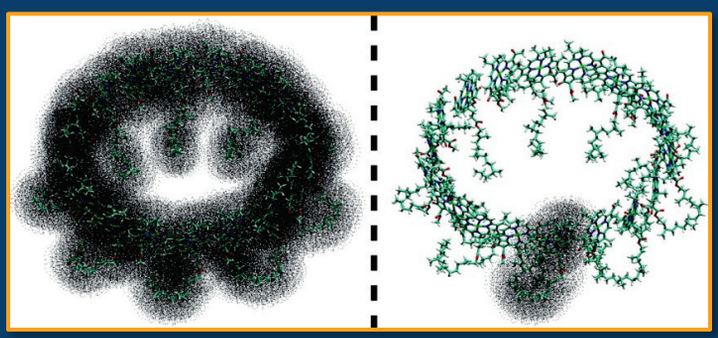
Scientific Computing & Modelling

Quality **Software**.
Quantum **Science**.

Excitons and Electronic Transport in ADF

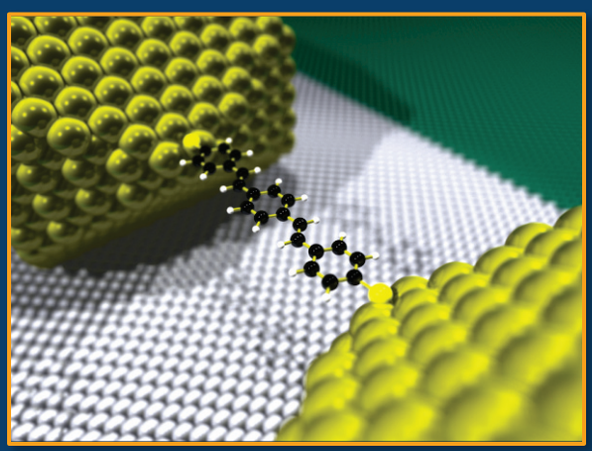
Excitations with TDDFT

- Spin-orbit coupling
- Environment effects
- Excitonic coupling: FDEc, DIM/QM
- Excited state optimization
- State-selective excitations
- Franck-Condon factors
- Resonance Raman scattering
- Life-time effects
- Model XC: SAOP, GRAC, LB94
- Slater orbitals: correct behavior
- TDCDFT: Vignale-Kohn functional
- Periodic TDDFT: dielectric function, EELS



Electronic transport

- Transfer integrals
- Non-equilibrium Green's functions
- Charge-localized states with FDE(m)



General

- Expert staff and support
- Latest developments
- Integrated GUI: prepare, run, analyze
- Accurate relativistic effects
- Strong in spectroscopy and analysis

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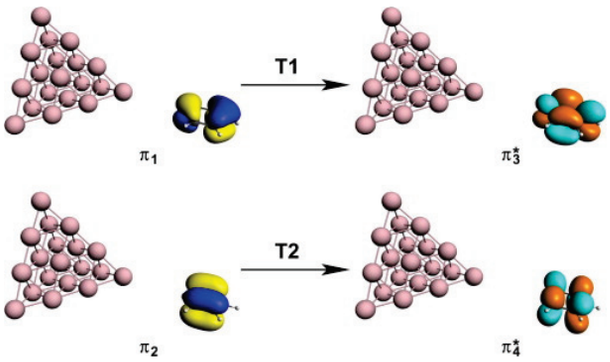
Exciton & Charge Transfer Modeling Research Highlights

Scientific Computing & Modelling

State-selective excitations with subsystem TDDFT (FDEc): exciton coupling on excited state potential energy surfaces



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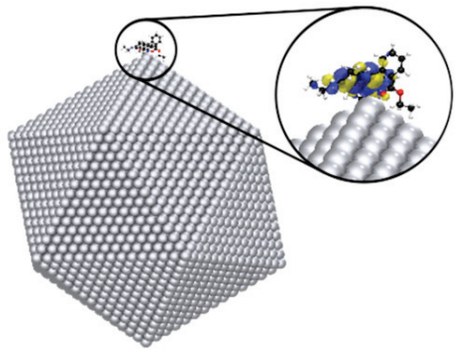
DIM/QM for molecules adsorbed on large nano-particles: plasmon-exciton hybridization, surface-enhanced Raman



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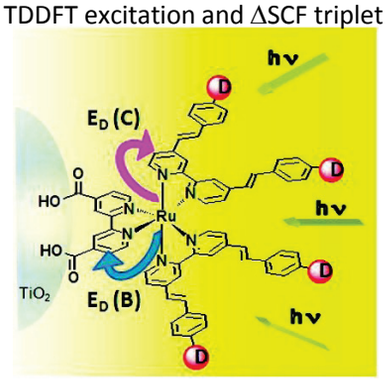
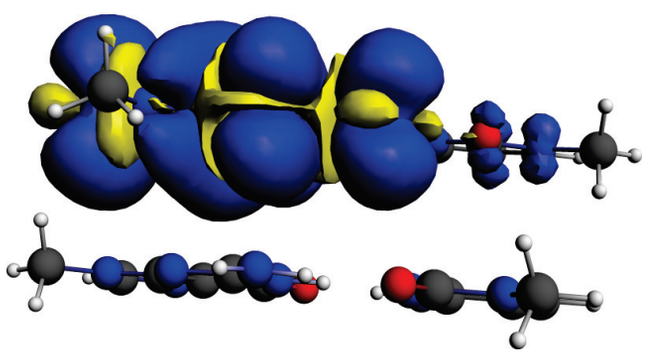
Dye-Sensitized Solar Cell efficiency: estimate electron injection with TDDFT excitation and ΔSCF triplet energies



F. Gajardo, M. Barrera, R. Vargas, I. Crivelli, B. Loeb, *Influence of the Nature of the Absorption Band on … Ruthenium(II) Polypyridinic Complexes As Dyes for Sensitized Solar Cells*. Inorg. Chem. **50**, 5910-5924 (2011)

Charge localization from diabatic states with FDE(m) to calculate electronic coupling in hole transfers in B-DNA (GT+)



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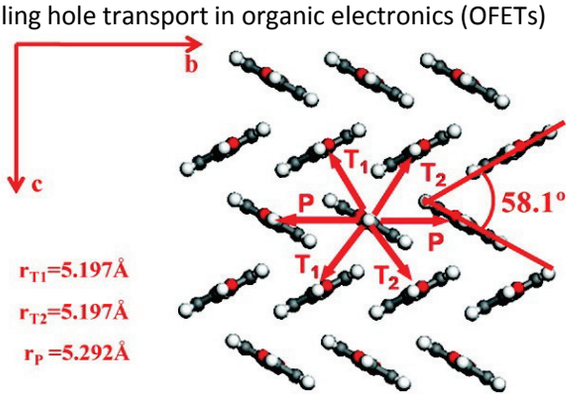
Charge transfer integrals from molecular fragments for modeling hole transport in organic electronics (OFETs)



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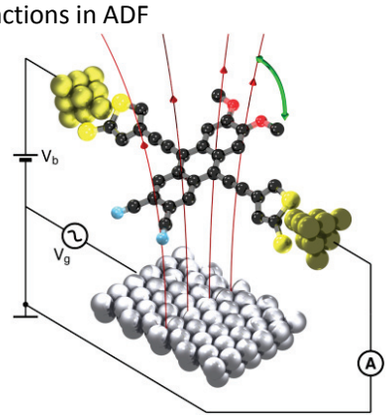
All-electric single-molecule motor with non-self-consistent Green's functions in ADF



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