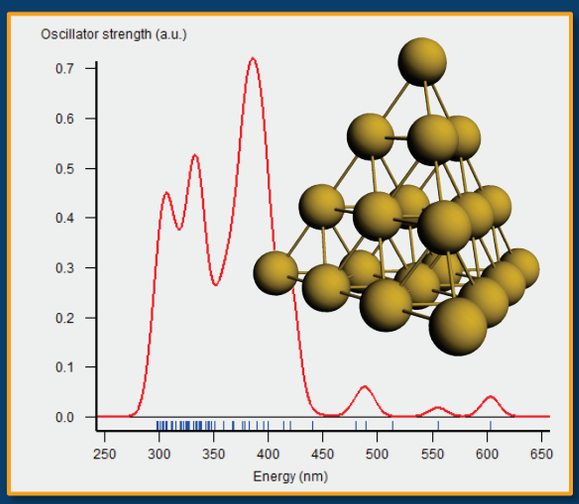
Scientific Computing & Modelling

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

Modeling Nanomaterials with ADF

Excitations with TDDFT

- Exciton coupling nanoparticle-adsorbate
  - TDDFT-atomistic electrodynamics
  - Coupled Frozen-Density Embedding
- State-selective excitations
- Core excitations
- Spin-orbit coupling
- Slater orbitals: correct behavior
- Model xc potentials

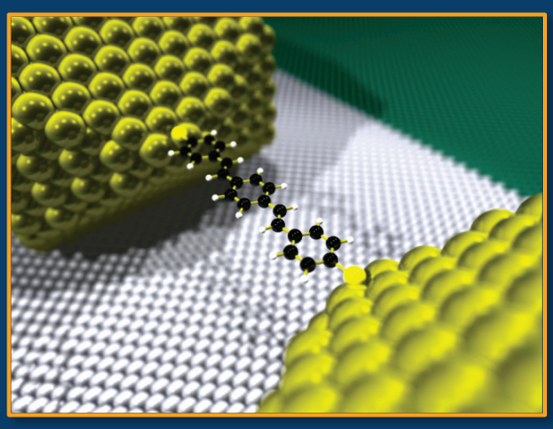


Integrated GUI and tools

- Easy switching periodic – molecular DFT
- Prepare, run, and analyze cross-platform
- Quickly set up multi-layer calculations

Electronic transport

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



General

- Expert staff and support
- Latest developments
- Accurate relativistic effects
- Strong in spectroscopy and analysis

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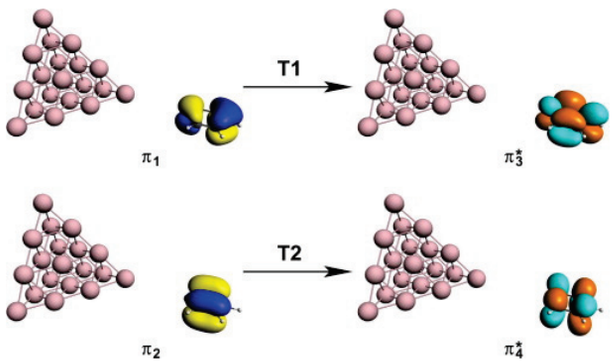
Nanomaterials Modeling Research Highlights

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



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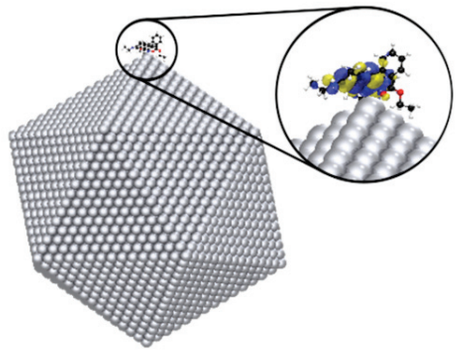
DIM/QM for molecules adsorbed on large nano-particles: plasmon-exciton hybridization, surface-enhanced Raman



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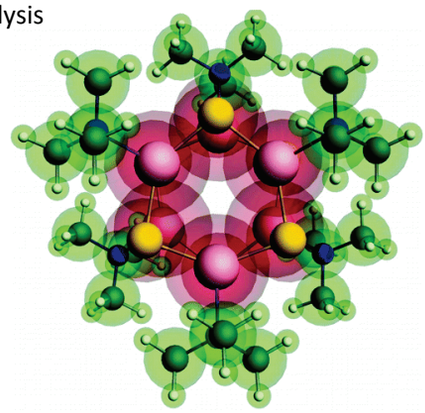
Passivated ZnS Quantum Dots with QM/MM: structural and bonding analysis



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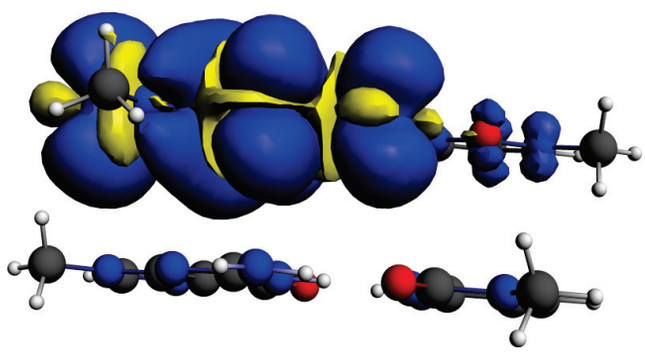
Charge localization from diabatic states with FDE(m) to calculate electronic coupling in hole transfers in B-DNA (GT+)



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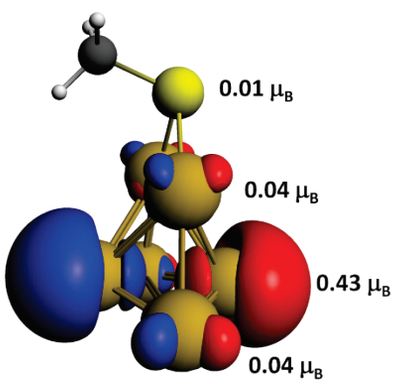
Sulphur-passivation affects magnetism of gold clusters: spin polarization pushed to outer Au atoms by thiolate



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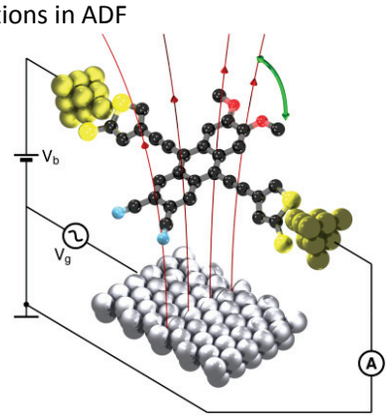
All-electric single-molecule motor with non-self-consistent Green's functions in ADF



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