Scientific Computing & Modelling

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

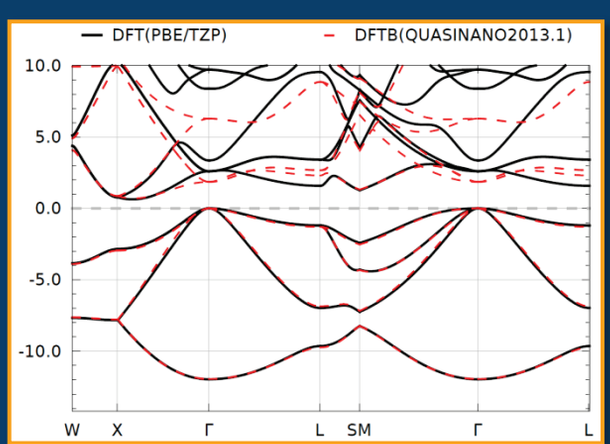
ADF Suite for Materials Modeling

Organic Electronics

- OLEDs: phosphorescent lifetimes with SO-TDDFT
- OFETs: electron / hole mobility with charge transfer integrals
- DSSCs: absorption, electron injection, dye regeneration
- NEGF (ADF, BAND, DFTB): single-molecule transport

BAND: periodic DFT

- Properties: BS, (p)DOS, AIM, ELF, MOs, EELS, NMR, ESR, EFG, phonons
- Band gap engineering (mBJ, GLLB-sc)
- True 2D periodicity (E fields, solvation)
- Relativity: Scalar, Spin-Orbit

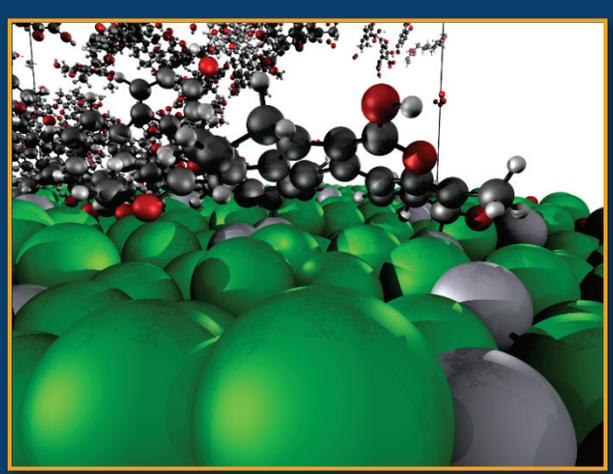


DFTB: fast, approximate DFT

- Molecules and periodic (1D, 2D, 3D)
- MD, phonons, many properties
- Electronic parameters for most elements

ReaxFF: Reactive Molecular Dynamics

- GUI: prepare , run,analyze reactions
- Semi-automatic parameterization
- Accelerated MD, T regimes, constraints



Fast and easy modeling suite

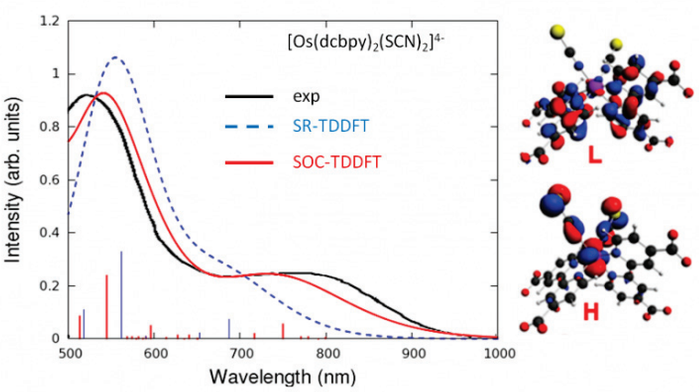
- Parallel install out of the box
- Integrated Graphical interface
- Expert staff and support

www.scm.com

Scientific Computing & Modelling

Materials Modeling Research Highlights

Spin-orbit coupling boosts dye-sensitized solar cell efficiency



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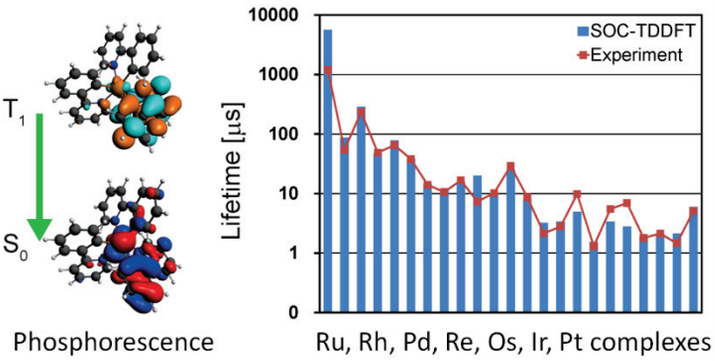
Predicting Phosphorescence lifetimes for OLED emitters



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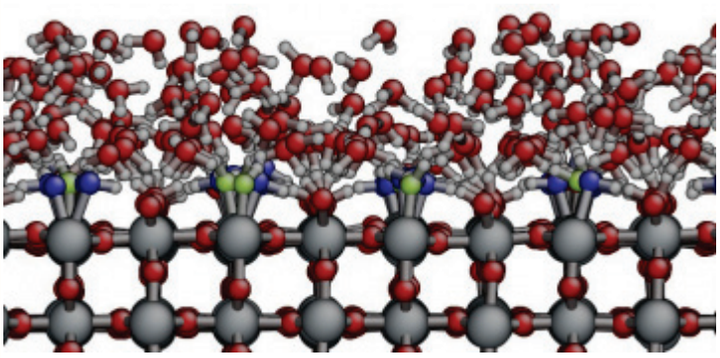

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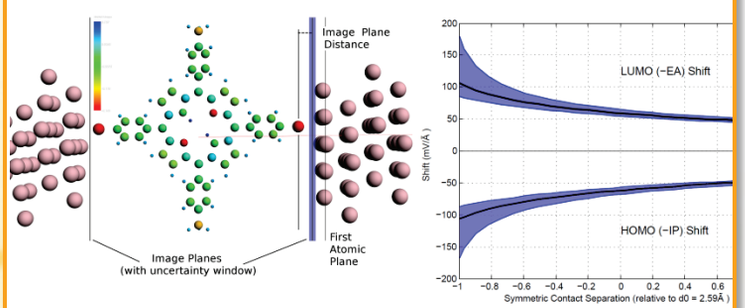

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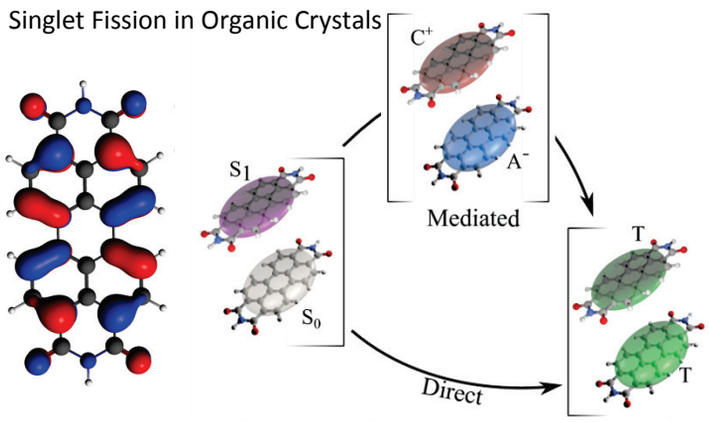
Singlet Fission in Organic Crystals



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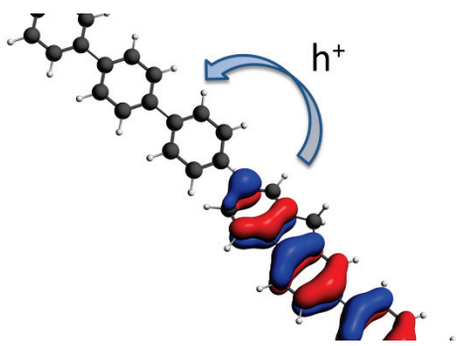

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