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
Materials Modeling Research Highlights

Spin-orbit coupling boosts dye-sensitized solar cell efficiency


Water absorption and dissociation on TiO₂ surfaces


Singlet Fission in Organic Crystals


Environment effect on hole mobility in organic polymers


Predicting Phosphorescence lifetimes for OLED emitters


Self-consistent NEGF explains break-through experiment on mechanical and electrostatic effects on molecular transport


Free ADF demo license: [www.scm.com/trial](http://www.scm.com/trial)