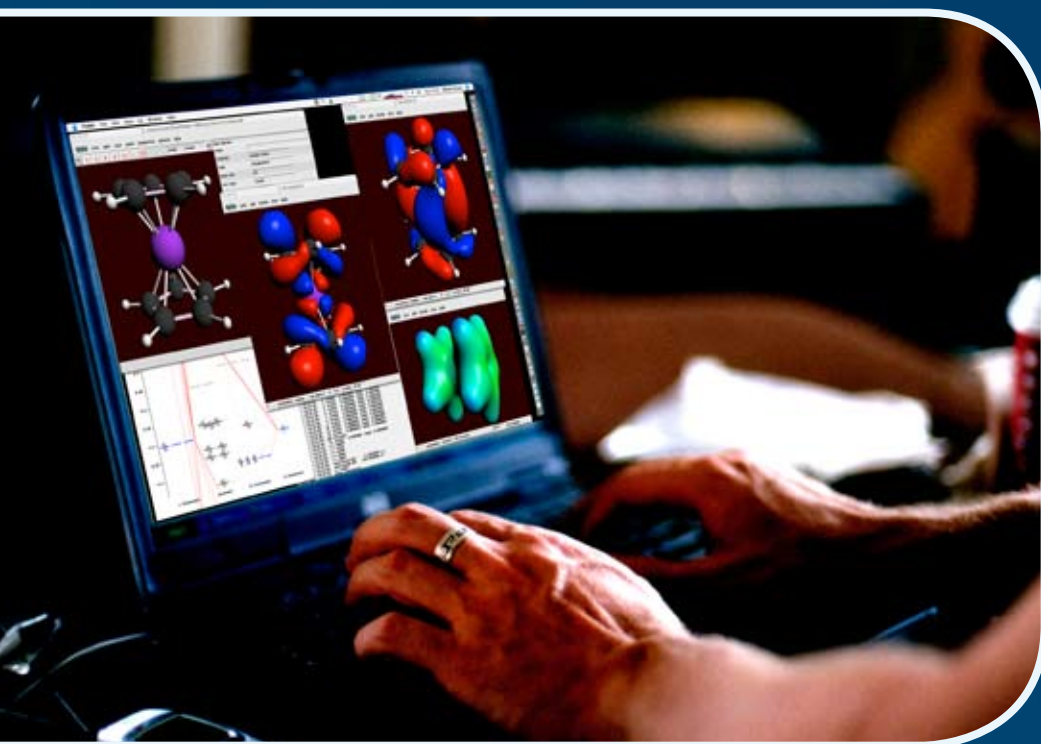


ADF 2006

*The universal
density functional
package for chemists!*



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Feature list

The molecular ADF program

- **Geometry optimizations, transition states, and reaction paths**
 - GO, TS searches (eigenvector following, NEB), IRC, LT, (analytical) frequencies
 - initial Hessian estimate, constraints, restraints possible
 - Cartesian, internal and delocalized coordinates
- **Model Hamiltonians**
 - XC energies: LDA, GGA, hybrids (like B3LYP), meta-GGA
 - potentials: LDA, GGA, hybrids, SAOP, GRAC, LB94; forces: LDA, GGA
 - relativistic effects (ZORA and spin-orbit coupling during SCF)
 - solvents and other environments: COSMO, QM/MM, DRF, DFT/DFT
 - homogeneous electric field, point charges
- **Molecular properties**
 - UV/Vis spectra, open-shell, closed shell, spin-orbit coupled, oscillator strengths
 - core excitations, X-ray absorption spectra
 - frequency-dependent (hyper-)polarizabilities (nonlinear optics)
 - (resonance) Raman, dispersion coefficients
 - CD rotatory strengths, ORD (chiral molecules)
 - NMR chemical shifts, spin-spin couplings
 - ESR (EPR) g-tensors, hyperfine interactions, A-tensors, NQCC (EFG)
 - IR
- **Analysis ("DFT is a quantitative MO theory")**
 - molecule built from fragments
 - bond energy analysis
 - Mulliken, Voronoi, and Hirshfeld charges, bondorders, NBO
 - molecular symmetry: T_d , O_h , C_i , C_s , C_n , C_{nv} , C_{nh} , D_n , D_{nv} , D_{nh} etc.
- **Accuracy and Efficiency**
 - Slater type basis sets
 - $Z = 1$ to 118, all electron, frozen-core, nonrelativistic and relativistic
 - SZ, DZ, DZP, TZP, TZ2P, QZ4P, even-tempered, diffuse
 - te Velde-Baerends integration scheme
 - parallelization
 - density fit, linear scaling techniques, distance cut-offs

The periodic BAND program

- bulk crystals, polymers, surfaces
- XC energies and potentials: LDA, GGA
- relativistic effects (ZORA and spin-orbit coupling)
- numerical orbitals and Slater type basis sets
- TDDFT - frequency-dependent dielectric functions, EELS
- DOS (total, partial, population), Mulliken population analysis, form factors
- bond energy analysis, fragment approach possible

The ADF-GUI and the BAND-GUI

- ADFinput, BANDinput - draw or import molecule, select options, start ADF or BAND calculation
- ADFview - visualize 3D data fields for orbitals, densities, potentials, etc. for ADF and BAND
- ADFspectra - visualize density-of-states, IR, Raman, CD, or optical spectra for ADF
- BANDstructure - shows plot of the electronic band structure
- ADFlevels - draws interaction diagram for ADF
- ADFmovie - shows normal mode vibrations or steps in optimization for ADF
- ADFtail - shows a summary of the progress of an ADF or BAND calculation
- BOB - basic output browser for ADF and BAND

*Supported Platforms:
Windows, Mac OS X, major Linux and UNIX platforms*



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