Scientific Computing & Modelling

ADF-GUI Quick Reference Manual

ADF Program System
Release 2010

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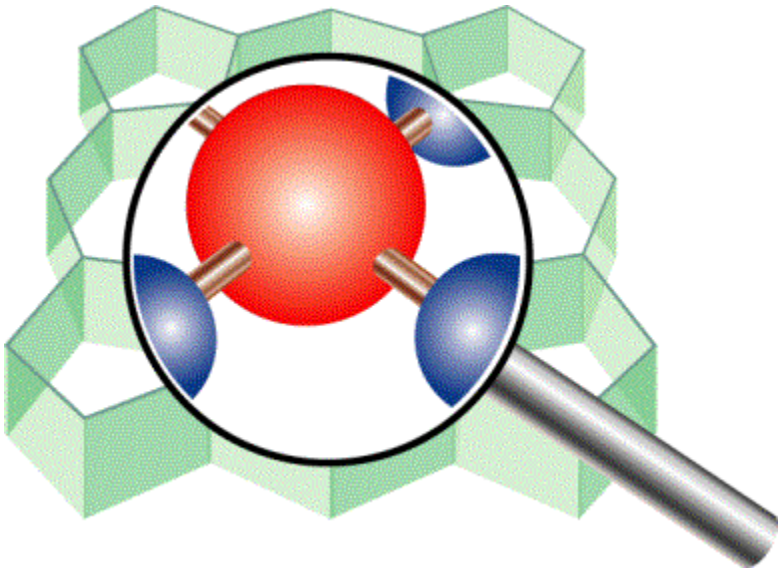

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Introduction

This document will provide a quick reference manual of the ADF-GUI. ADF-GUI is the Graphical User Interface for the ADF package.
If you are new to the ADF-GUI we advise you to study the ADF-GUI tutorial.

The ADF-GUI modules

- ADFjobs - mangages ADF jobs
- ADFinput - builds the input for an ADF calculation
- ADFview - displays 3-D (volume) data, such as electron densities, orbitals, electrostatic potentials
- ADFspectra - shows spectra calculated by ADF, like IR and excitation spectra
- ADFmovie - follows geometry steps of geometry optimizations, IRC calculations, etc
- ADFlevels - shows energy diagram
- ADFdos - shows density-of-states graphs
- ADFtail - follows the progress of an ADF calculation
- ADFoutput - browses the output generated by ADF
- GUIprefs - changes preferences that are being used by the ADF-GUI

The modules can be started from $ADFBIN or from a different module using the SCM menu.

module	**$ADFBIN**	**file extension**	**SCM menu**
ADFjobs	adfjobs		Jobs
ADFinput	adfinput	.adf	ADF Input
ADFview	adfview	.t21 .t41	View
ADFspectra	adfspectra	.t21	Spectra
ADFmovie	adfmovie	.amv .logfile .t21	Movie
ADFlevels	adflevels	.t21	ADF Levels
ADFdos	adfdos	.t21	Dos
ADFtail	adftail	.logfile	Logfile
ADFoutput	adfoutput	.out	Output
GUIprefs	guiprefs		Preferences

Mouse Interaction

A one-button mouse button is the same as a Left mouse button

Rotate	Left
Rotate in-plane	Ctrl-Left
Translate	Middle, or Alt-Left
Zoom	Right, or Command-Left (drag up or down), or use the scroll wheel on your mouse
New selection	Click on an object
Clear selection	Click in space
Add or remove selection	Shift-Click on object
Add all objects within rectangle	Shift-Drag in space

Build the molecule

`ADFinput drawing area`

Import Coordinates: Select **File** → **Import Coordinates ...**.
Add atom: Select an atom-tool by clicking on the button with the 'C', 'O', 'N', 'H', 'Cl', or 'X' (popup menu showing all elements).
Click somewhere in the drawing area to draw the atom.
Add hydrogens: Select **Atoms** → **Add Hydrogen**.
Add structure: Select a structure from the Structures' Menu (the button with a benzene molecule).
Click somewhere in the drawing area to place the structure. Double-click on an atom to replace it with the structure. Use the **Atoms** → **Replace By Structure** to replace all atoms in a selection by structures.
Predefined Structures can be found for: Alkyl Chains, Aromatic Molecules, Cyclic Hydrocarbons, Ligands, Polyhedra, Amino Acids, parts of DNA, Metal Complexes, Solvents.
Change atom (bond) type: Select the atom (bond).
Select **Atoms** → **Change Atom Type** (**Bonds** → **Bond Order**).
Guess bonds: Select **Bonds** → **Guess bonds**.
Delete atoms: Select **Atoms** → **Delete Atom(s)**.
Edit commands: Select **Edit** → **Copy**, **Edit** → **Paste**, **Edit** → **Select**, ..., etc.
Undo: Select **Edit** → **Undo** to go back in time.

`Pre-optimization of the geometry`

ADFinput: Click on the Optimizer button (the gear button), simple MM. Open the right panel and select the desired method for pre-optimization (such as DFTB, Mopac, Open Babel). Example **Right Panel** → **DFTB** → **Run**. Whether or not the requested method works, depends also on whether the requested program has been installed or whether or not the required parameter files are present.
ADFUsersGuide: DFTB [1]
ADFGUIReference: preoptimizers [1]

Run the ADF calculation

ADFinput: Build the molecule and select the desired options. Select **File** → **Save**. Enter a name in the File name field. Select **File** → **Run**.

Atoms, Basis sets

`Slater type basis sets, density fit and frozen core approximation`

> **ADFinput:** Select **Right Panel** → **Main Options**. Select the basis set from the 'Basis Set' Menu. Select the frozen core from the 'Core Type' Menu.
> **ADFUsersGuide:** STO [1,2], density fit [1], frozen core approximation [1].

`Ghost atoms, Alternative elements, expert atomic options`

> **ADFinput:** Click on an atom (or selection), **Atoms** → **Ghosts** → **Change Atoms To Ghosts**.
> **ADFinput:** Alternative elements, expert atomic options: Select **Atoms** → **Atom Details**. Move the mouse over the check buttons to see a help balloon which will give you details on what it is, and on how to change it.
> **ADFUsersGuide:** Ghost atoms, alternative elements [1].

`Nuclear Model`

> **ADFinput:** Select **Right Panel** → **Relativity**. Select 'PointCharge' or 'Gaussian' (finite size nucleus) for 'Nuclear Model'.
> **ADFUsersGuide:** nuclear model [1].

Model Hamiltonians

`XC energy functionals and potentials`

> **ADFinput:** Select **Right Panel** → **Main Options** and select the desired SCF potential for 'XC potential in SCF'. Select for METAGGA or hybrid functional energies after SCF the corresponding box
> **ADFUsersGuide:** XC [1].

`Relativistic effects (ZORA and spin-orbit coupling)`

> **ADFinput:** Select **Right Panel** → **Main Options**. Select 'None', 'Scalar, or 'Spin-Orbit' for 'Relativity'.
> **ADFUsersGuide:** relativity [1].

`Solvents and other environments`

> **ADFinput:** COSMO, SCRF: Select **Right Panel** → **Solvation**. Select the desired method for 'Solvation method'. Select the desired solvent for 'Solvent'.
> **ADFinput:** FDE, QM/MM, Quild: **Right Panel** → **FDE**, **Right Panel** → **QMMM**, **Right Panel** → **Quild**.
> **ADFinput:** DRF, 3D-RISM: no direct GUI support.
> **ADFGUIReference:** multi-level methods, FDE, QM/MM, Quild [1]
> **ADFUsersGuide:** COSMO [1], SCRF [1], QM/MM [1,2], DRF [1], FDE [1], 3D-RISM [1], Quild [1].

`Homogeneous electric field and point charges`

> **ADFinput:** Select **Right Panel** → **Electric field**. Enter the values of the homogeneous electric field in the menu 'Electric field - '. Enter the coordinates and values of the point charges in the text box.
> **ADFUsersGuide:** EField [1]

Structure and Reactivity

`Geometry Optimizations, Transition State searches, Intrinsic Reaction Coordinates, Linear Transit`

> **ADFinput:** Select **Right Panel** → **Main Options**. Select 'Geometry Optimization', 'Transition State Search', 'IRC', or 'Linear Transit' in the 'Preset' menu.
> **ADFmovie:** follow the steps in the geometry .
> **ADFUsersGuide:** geometry optimization [1], TS [1,2], IRC [1], LT [1].

`Excited state (geometry) optimizations`

> See section on excited state (geometry) optimizations.

`Optimizations in Cartesian, internal, and delocalized coordinates`

> **ADFinput:** Select **Right Panel** → **Coordinates'**. Select 'Cartesian', 'Internal', or 'Delocalized' from the 'Use ... coordinates' menu.
> **ADFUsersGuide:** coordinates [1].

`Frequencies`

> See section on vibrational spectroscopy.

`Constraints`

> **ADFinput:** Select **Right Panel** → **Coordinates**. To freeze a coordinate: check the corresponding box in the list of atoms.
> **ADFinput:** Select **Right Panel** → **Geometry Constraints and Scan**. To freeze distance, angle or dihedral: select 2, 3, or 4 atoms with the mouse and add constraint.
> **ADFUsersGuide:** constraints [1,2,3].

Spectroscopic properties

If possible do a molecular property in a single point run.
ADFoutput: Browse the output to find the values (scalars, vectors, tensors) of the calculated property.

`Vibrational spectroscopy`

`IR frequencies and intensities`

> **ADFinput:** Select **Right Panel** → **Main Options**. Select the 'Frequencies' in the 'Preset' menu.
> **ADFspectra:** Select 'Vibration' from the 'Spectra' Menu. Move Mouse above the spectrum to get more information in a popup menu. Select mode for visualization with ADFmovie.
> **ADFUsersGuide:** IR [1].

`(Resonance) Raman`

> **ADFinput:** Select **Right Panel** → **Main Options**. Select the 'Frequencies' in the 'Preset' menu.
> Raman: Select **Right Panel** → **Raman, VROA**. Select 'Raman Full' for 'Calculate:'.
> Resonance Raman: Select **Right Panel** → **Raman, VROA**. Select 'Raman Full AORESPONSE' for 'Calculate:'. Enter a resonance peak width (in hartree).
> **ADFspectra:** Select **Spectra** → **Raman**. Move Mouse above the spectrum to get more information in a popup menu.
> **ADFUsersGuide:** Raman [1], Resonance Raman [1].

Vibrational Circular Dichroism (VCD)

ADFinput: Select **Right Panel** → **Main Options**. Select the 'Frequencies' in the 'Preset' menu. Next select **Right Panel** → **VCD**. Select the checkbox 'calculate VCD intensities **ADFspectra:** Select **Spectra** → **VCD**. Move Mouse above the spectrum to get more information in a popup menu.
ADFUsersGuide: VCD [1].

Time-dependent DFT

ADFUsersGuide: TDDFT [1].

UV/Vis spectra, oscillator strengths, open shell excitations, core excitations

ADFinput: Select **Right Panel** → **Excitations, CD**. Select, for example, the checkbox 'SingletAndTriplet'.
ADFspectra: Select **Spectra** → **Excitation**. Move Mouse above the spectrum to get more information in a popup menu.
ADFUsersGuide: UV/Vis spectra, oscillator strengths [1], open shell excitations [1], core excitations [1].

Excited state (geometry) optimizations

ADFinput: Select **Right Panel** → **Main Options**. Select 'Geometry Optimization', 'Transition State Search', 'IRC', or 'Linear Transit' in the 'Preset' menu.
Select **Right Panel** → **Excitations, CD**. Select, for example, the checkbox 'SingletAndTriplet'.
Select **Right Panel** → **Ecxited State Geometry**. Enter the requested excitation, like 2B1.u or 3A (name irreps depend on actual symmetry).
ADFUsersGuide: excited state optimizations [1].

frequency-dependent polarizabilities

ADFinput: Select **Right Panel** → **Polarizability**. Select the checkbox 'Calculate Polarizability'.
ADFUsersGuide: polarizabilities [1].

frequency-dependent hyperpolarizabilities

ADFinput: Select **Right Panel** → **Hyperpolarizability**. Select the checkbox 'Calculate Hyperpolarizability'.
ADFUsersGuide: polarizabilities [1].

van der Waals dispersion coefficients

ADFinput: Select **Right Panel** → **VanderWaals**. Select the checkbox 'Calculate Van der Waals dispersion coefs'.
ADFUsersGuide: dispersion [1,2].

Rotatory strengths (CD) and optical rotatory dispersion (ORD)

ADFinput: CD spectrum: Select **Right Panel** → **Excitations, CD**. Select the checkbox 'Calculate rotatory strengths (CD)'. Select, for example, the checkbox 'SingletAndTriplet'.
ADFspectra: CD: Select **Spectra** → **CD**. Move Mouse above the spectrum to get more information in a popup menu.
ADFinput: ORD: Select **Right Panel** → **Optical Rotation Dispersion**. Select the checkbox 'Calculate Optical Rotation'.
ADFUsersGuide: CD [1], ORD [1].

Magnetizability

ADFinput: Select **Right Panel** → **Magnetizability, Verdet**. Select 'Magnetizability' for 'Calculate'.
ADFUsersGuide: magnetizability [1]

`magnetic circular dichroism (MCD) and Verdet constants`

ADFinput: MCD spectrum: Select **Right Panel** → **MCD**. Select the required terms (A, B, C) for 'Calculate MCD'.
ADFspectra: MCD: Select **Spectra** → **MCD**. Move Mouse above the spectrum to get more information in a popup menu.
ADFinput: Select **Right Panel** → **Magnetizability, Verdet**. Select 'VerdetConstant' for 'Calculate'.
ADFUsersGuide: MCD [1], Verdet constants [1].

`NMR chemical shifts, spin-spin couplings`

ADFinput: Select **Right Panel** → **NMR**. Select the checkbox 'Isotropic Shielding Constants' or 'Shielding Tensor', or Select the checkbox 'Calculate spin-spin coupling constants'.
ADFUsersGuide: chemical shifts [1,2], spin-spin couplings [1].

`ESR (EPR) g-tensor, A-tensor`

ADFinput: Select **Right Panel** → **ESR, EPR, EFG'**. Select the checkbox 'ESR g-tensor/A-tensor'.
ADFUsersGuide: ESR [1,2].

`Nuclear quadrupole coupling constants, EFG, ESR Q-tensor, quadrupole splittings`

ADFinput: Select **Right Panel** → **ESR, EPR, EFG**. Select the checkbox 'EFG Q-tensor'.
ADFUsersGuide: EFG [1].

`Mössbauer isomer shifts`

ADFinput: No special input needed.
ADFoutput: Electron Density at nucleus.
ADFUsersGuide: Mössbauer [1].

Analysis

If possible do the analysis in a single point run.
ADFoutput: Browse the output to find the complete analysis.

`Fragments`

ADFinput: Select **Right Panel** → **Fragments** to use a fragment analysis. Select **Right Panel** → **Regions** to define the fragments. Select all atoms that form a fragment. Press the '+' button to add a fragment.
ADFGUIReference: fragments [1] **ADFUsersGuide:** fragments [1].

`Bond energy analysis`

ADFinput: No special input is needed.
ADFUsersGuide: bond energy analysis [1].

`ETS-NOCV analysis`

ADFinput: Select **Right Panel** → **ETS-NOCV**. Select 'Closed Shell' or 'Open Shell' for 'ETS-NOCV Analysis'.
ADFUsersGuide: ETS-NOCV [1].

`Advanced charge density and MO analysis`

ADFinput: Mulliken, VDD, Hirshfeld, MDC, MO Analysis: No special input is needed.
ADFinput: Bader Analysis: Select **Right Panel** → **Other: Etot, Bader, Charge Transport**. Select the checkbox 'calculate Bader Atomic Properties'.
ADFinput: NBO Analysis: Select **Right Panel** → **Orbitals**. Select the checkbox 'Perform NBO Analysis'.
ADFlevels: Energy diagram.
ADFview: Electron densities, potentials, MOs, ELF, etc.
ADFdos: Select an atom to see a GPDOS. Select an atom and hold the mouse for a popup menu to select the GPDOS for S, P, D, or F functions.
ADFspectra: Select **Spectra** → **DOS**.
ADFUsersGuide: Mulliken [1], Hirshfeld and Voronoi deformation density [1], Bondorders [1], Bader [1], NBO [1].

`Molecular symmetry`

ADFinput: Possibility to symmetrize the molecule with the Symmetry button (the five-point star button).
ADFUsersGuide: symmetry [1,2].

`Charge transfer integrals (transport properties)`

ADFinput: Typically use 2 fragments. Select **Right Panel** → **Symmetry**. Select 'NOSYM' for the 'Symbol'. Select **Right Panel** → **Other: Etot, Bader, Charge Transport**. Select the checkbox 'Charge transfer integrals (for transport properties)'.
ADFUsersGuide: transfer integrals [1].

Accuracy and Efficiency

`Slater type basis sets, density fit and frozen core approximation`

See section on basis sets.

`Integration scheme`

ADFinput: Select **Right Panel** → **Main Options**. Enter the value for the accuracy of the integration grid in the menu 'Integration Accuracy'.
ADFUsersGuide: accuracy [1].

`Parallelization`

ADFjobs: See ADF-GUI Reference Manual.
ADFUsersGuide: parallelization [1].

`Linear scaling / distance cut-offs`

ADFinput: Select **Right Panel** → **Technical**. **ADFUsersGuide:** linear scaling [1].

`SCF convergence`

ADFinput: Select **Right Panel** → **SCF** or **Right Panel** → **SCF Convergence Aids**. **ADFUsersGuide:** Sections 2.8 and 3.2 [1].

Scripting

`Prepare (multiple) ADF jobs`

ADFjobs: 'Prepare...' from the 'Tools' Menu.
ADFUsersGuide: ADFprep [1].

`Generate report`

ADFjobs: Select 'Build ... Report ' from the 'Tools' Menu.
ADFUsersGuide: ADFreport [1].

Tips

- Tear off field pull-down menus in ADFview
- Tear off normal mode menus in ADFspectra
- Structure Tool: Double click on atom to replace it with a structure
- Structure Tool: Click in empty space and connect the structure to an atom
- Structure Tool: The Spacebar sets the last used Structure too
- Your own structures: save the .adf file in the $SCM_STRUCTURES folder
- Make use of 'set origin' and dummy atoms when making your own structures
- The help menu offers a direct link to the online tutorial for ADF-GUI
- The help menu offers a direct link to the ADF reference manual
- Change the default background color for all GUI-modules in your preferences
- Use the SCM menu (the logo)
- Zoom: drag the mouse up or down holding the right button or command-left
- Translate: drag the mouse while holding the middle button or alt-left
- Rotate: drag the mouse while holding the left button
- Rotate in Plane: drag the mouse while holding the ctrl-key
- Rotate Selection: drag while holding the mouse button down on the selection
- Select using shift-drag in space will select all atoms within the rectangle
- Use Anti-Alias to save high quality pictures (slow ...)
- Save your default calculation setup by using the templates
- Use the PropertiesOnly preset to avoid re-calculation
- Use the None preset to save only yellof fields in a preset
- Use the atom toolbuttons and doubleclick to change the chosen atom
- The C-key sets the Carbon tool
- The H-key sets the Hydrogen tool
- The N-key sets the Nitrogen tool
- The O-key sets the Oxygen tool
- The F-key sets the Fluorine tool
- The P-key sets the Phosphorus tool
- The S-key sets the Sulfur tool
- The Esc-key sets the Pointer tool
- The 1-key sets the single-bond mode
- The 2-key sets the double-bond mode
- The 3-key sets the triple-bond mode
- The 4-key sets the aromatic-bond mode
- Add hydrogen works on all available sites if you have no atoms selected
- Constrain bond lengths while building? Toggle this option in the Bonds menu
- Bond Length: Select two atoms and, if possible, change the bond length
- Bond Angle: Select three atoms and, if possible, change the angle
- Dihedral Angle: Select four atoms and, if possible, change the angle
- Plane angle: Select five atoms that define two planes and change the angle
- Change the order of the atoms in the coordinates panel
- Changing the order of the atoms will affect the internal coordinates
- Deleting or adding bonds will affect the internal coordinates
- Use the User Input field to add anything you like to the ADF input file
- Double click the .run file in ADFjobs to edit it