



Gaussian 16 Features at a Glance

Features introduced since Gaussian 09 Rev A are in **blue**.
Existing features enhanced in Gaussian 16 are in **green**.

Fundamental Algorithms

- ♦ Calculation of one- & two-electron integrals over any contracted gaussian functions
- ♦ Conventional, direct, semi-direct and in-core algorithms
- ♦ Linearized computational cost via automated fast multipole methods (FMM) and sparse matrix techniques
- ♦ Harris initial guess
- ♦ Initial guess generated from fragment guesses or fragment SCF solutions
- ♦ Density fitting and Coulomb engine for pure DFT calculations, including automated generation of fitting basis sets
- ♦ $\mathcal{O}(N)$ exact exchange for HF and hybrid DFT
- ♦ 1D, 2D, 3D periodic boundary conditions (PBC) energies & gradients (HF & DFT)
- ♦ Shared-memory (SMP), cluster/network and **GPU-based** parallel execution

Model Chemistries

Molecular Mechanics

- ♦ Amber, DREIDING and UFF energies, gradients and frequencies
 - * Custom force fields
- ♦ Standalone MM program

Ground State Semi-Empirical

- ♦ CNDO/2, INDO, MINDO3 and MNDO energies and gradients
- ♦ AM1, PM3, PM3MM, PM6 and PDDG energies, gradients and reimplemented (analytic) frequencies
- ♦ **PM7: original and modified for continuous potential energy surfaces**
- ♦ Custom semi-empirical parameters (Gaussian and MOPAC External formats)
- ♦ DFTB and DFTBA methods

Self Consistent Field (SCF)

- ♦ SCF restricted and unrestricted energies, gradients and frequencies, and RO energies and gradients
- ♦ **EDIIS+CDIIS default algorithm; optional Quadratic Convergent SCF**
- ♦ **SCF procedure enhancements for very large calculations**
- ♦ Complete Active Space SCF (CASSCF) energies, gradients & frequencies
 - * Active spaces of up to **16** orbitals
- ♦ Restricted Active Space SCF (RASSCF) energies and gradients
- ♦ Generalized Valence Bond-Perfect Pairing energies and gradients
- ♦ Wavefunction stability analysis (HF & DFT)

Density Functional Theory

Closed and open shell energies, gradients & frequencies, and RO energies & gradients are available for all DFT methods.

- ♦ EXCHANGE FUNCTIONALS: Slater, Xa, Becke 88, Perdew-Wang 91, Barone-modified PW91, Gill 96, PBE, OPTX, TPSS, **revised TPSS**, BRx, PKZB, ω PBEh/HSE, PBEh
- ♦ CORRELATION FUNCTIONALS: VWN, VWN5, LYP, Perdew 81, Perdew 86, Perdew-Wang 91, PBE, B95, TPSS, **revised TPSS**, KCIS, BRC, PKZB, VP86, V5LYP
- ♦ OTHER PURE FUNCTIONALS: VSXC, HCTH functional family, τ HCTH, B97-D, M06-L, SOGGA11, M11-L, MN12-L, N12, **MN15-L**
- ♦ HYBRID METHODS: B3LYP, B3P86, P3PW91, B1 and variations, B98, B97-1, B97-2, PBE1PBE, HSEh1PBE and variations, O3LYP, TPSSh, τ HCTH hybrid, BMK, **AFD**, M05, M05-2X, M06, M06-HF, M062-X, **M08-HX**, **PW6B95**, **PW6B95D3**, **M11**, **SOGGA11-X**, **N12**, **N12-SX**, **MN12-SX**, **MN15**, HISSbPBE, X3LYP, BHandHLYP; user-configurable hybrid methods
- ♦ DOUBLE HYBRID: B2PLYP & mPW2PLYP and variations with dispersion, **DSDPBEP86**, **PBE0DH**, **PBEQIDH** (see also below in "Electron Correlation")

- ♦ EMPIRICAL DISPERSION: **PFD**, **GD2**, **GD3**, **GD3BJ**
- ♦ FUNCTIONALS INCLUDING DISPERSION: **APFD**, **B97D3**, **B2PLYPD3**
- ♦ LONG RANGE-CORRECTED: LC- ω PBE, CAM-B3LYP, ω B97XD and variations, Hirao's general LC correction
- ♦ **Larger numerical integrations grids**

Electron Correlation:

All methods/job types are available for both closed and open shell systems and may use frozen core orbitals; restricted open shell calculations are available for MP2, MP3, MP4 and CCSD/CCSD(T) energies.

- ♦ MP2 energies, gradients, and frequencies
- ♦ **Double hybrid DFT** energies, gradients and frequencies, with optional empirical dispersion (see list in "Density Functional Theory" above)
- ♦ CASSCF calculations with MP2 correlation for any specified set of states
- ♦ MP3 and MP4(SDQ) energies and gradients
- ♦ MP4(SDTQ) and MP5 energies
- ♦ Configuration Interaction (CISD) energies & gradients
- ♦ Quadratic CI energies & gradients; QCISD(TQ) energies
- ♦ Coupled Cluster methods: restartable CCD, CCSD energies & gradients, CCSD(T) energies; optionally input amplitudes computed with smaller basis set
 - * **Optimized memory algorithm to avoid I/O during CCSD iterations**
- ♦ Brueckner Doubles (BD) energies and gradients, BD(T) energies; optionally input amplitudes & orbitals computed with a smaller basis set
- ♦ **Enhanced** Outer Valence Green's Function (OVGF) methods for ionization potentials & electron affinities
- ♦ Complete Basis Set (CBS) MP2 Extrapolation
- ♦ Douglas-Kroll-Hess scalar relativistic Hamiltonians

Automated High Accuracy Energies

- ♦ G1, G2, G3, G4 and variations
- ♦ CBS-4, CBS-q, CBS-QB3, ROCBS-QB3, CBS-Q, CBS-APNO
- ♦ W1U, W1BD, W1RO (**enhanced core correlation energy calculation**)

Basis Sets and DFT Fitting Sets

- ♦ STO-3G, 3-21G, 6-21G, 4-31G, 6-31G, 6-31G \dagger , 6-311G, D95, D95V, SHC, CEP- n G, LanL2DZ, cc-pV{D,T,Q,5,6}Z, original and def2- versions of SV, SVP, TZV & QZVP, EPR-II, EPR-III, Midi!, UGBS*, MTSmall, DG{D,T}ZVP, **CBSB7**
 - * **Augmented cc-pV*Z schemes: Aug- prefix, spAug-, dAug-, Truhlar calendar basis sets (original and regularized)**
- ♦ Effective Core Potentials (through second derivatives): LanL2DZ, CEP through Rn, Stuttgart/Dresden
- ♦ Support for basis functions and ECPs of arbitrary angular momentum
- ♦ DFT FITTING SETS: DGA1, DGA1, W06, older sets designed for SVP and TZVP basis sets; auto-generated fitting sets; optional default enabling of density fitting

Geometry Optimizations and Reaction Modeling

- ♦ Geometry optimizations for equilibrium structures, transition structures, and higher order saddle points, in redundant internal, internal (Z-matrix), Cartesian, or mixed internal and Cartesian coordinates
- ♦ **GEDIIS optimization algorithm**
- ♦ Redundant internal coordinate algorithm designed for large system, semi-empirical optimizations
- ♦ Newton-Raphson and Synchronous Transit-Guided Quasi-Newton (QST2/3) methods for locating transition structures
- ♦ IRCMax transition structure searches
- ♦ Relaxed and unrelaxed potential energy surface scans

- ◆ Implementation of intrinsic reaction path following (IRC), applicable to ONIOM QM:MM with thousands of atoms
- ◆ Reaction path optimization
- ◆ BOMD molecular dynamics (all analytic gradient methods); ADMP molecular dynamics: HF, DFT, ONIOM(MO:MM)
- ◆ Optimization of conical intersections via state-averaged CASSCF
- ◆ **Generalized internal coordinates for complex optimization constraints**

Vibrational Frequency Analysis

- ◆ Vibrational frequencies and normal modes (harmonic and **anharmonic**), including display/output limiting to specified atoms/residues/modes (optional mode sorting)
- ◆ Restartable analytic HF and DFT frequencies
- ◆ MO:MM ONIOM frequencies including electronic embedding
- ◆ Analytic Infrared and static and dynamic Raman intensities (HF & DFT; MP2 for IR)
- ◆ Pre-resonance Raman spectra (HF and DFT)
- ◆ Projected frequencies perpendicular to a reaction path
- ◆ NMR shielding tensors & GIAO magnetic susceptibilities (HF, DFT, MP2) and enhanced spin-spin coupling (HF, DFT)
- ◆ Vibrational circular dichroism (VCD) rotational strengths (HF and DFT; harmonic and **anharmonic**)
- ◆ Dynamic Raman Optical Activity (ROA) intensities (harmonic and **anharmonic**)
- ◆ **Raman and ROA intensities calculated separately from force constants in order to use a larger basis set**
- ◆ Harmonic vibration-rotation coupling
- ◆ **Enhanced** anharmonic vibrational analysis, including **IR intensities, DCPT2 & HDCPT2 method for resonance-free computations of anharmonic frequencies**
- ◆ Anharmonic vibration-rotation coupling via perturbation theory
- ◆ Hindered rotor analysis

Molecular Properties

- ◆ Population analysis, including per-orbital analysis for specified orbitals: Mulliken, **Hirshfeld/CM5**
- ◆ **Computed atomic charges can be saved for use in a later MM calculation**
- ◆ Electrostatic potential, electron density, density gradient, Laplacian, and magnetic shielding & induced current densities over an automatically generated grid
- ◆ Multipole moments through hexadecapole
- ◆ Biorthogonalization of MOs (producing corresponding orbitals)
- ◆ Electrostatic potential-derived charges (Merz-Singh-Kollman, CHelp, CHelpG, **Hu-Lu-Yang**)
- ◆ Natural orbital analysis and natural transition orbitals
- ◆ Natural Bond Orbital (NBO) analysis, including orbitals for CAS jobs. Integrated support for NBO3; **external interface to NBO6**
- ◆ Static and frequency-dependent analytic polarizabilities and hyperpolarizabilities (HF and DFT); numeric 2nd hyperpolarizabilities (HF; DFT w/ analytic 3rd derivs.)
- ◆ Approx. CAS spin orbit coupling between states
- ◆ Enhanced optical rotations and optical rotary dispersion (ORD)
- ◆ Hyperfine spectra components: electronic g tensors, Fermi contact terms, anisotropic Fermi contact terms, rotational constants, dipole hyperfine terms, quartic centrifugal distortion, electronic spin rotation tensors, nuclear electric quadrupole constants, nuclear spin rotation tensors
- ◆ ONIOM integration of electric and magnetic properties

ONIOM Calculations

- ◆ Enhanced 2 and 3 layer ONIOM energies, gradients and frequencies using any available method for any layer
- ◆ Optional electronic embedding for MO:MM energies, gradients and frequencies implemented so as to include all effects of the MM environment without neglecting terms in its coupling with the QM region
- ◆ Enhanced MO:MM ONIOM optimizations to minima and transition structures via microiterations including electronic embedding
- ◆ Support for IRC calculations
- ◆ ONIOM integration of electric and magnetic properties

Excited States

- ◆ ZINDO energies
- ◆ CI-Singles energies, gradients, & freqs.
- ◆ Restartable time-dependent (TD) HF & DFT energies, gradients and **frequencies. TD-DFT can use the Tamm-Dancoff approximation.**
- ◆ **SAC-CI energies and gradients**
- ◆ EOM-CCSD energies and **gradients** (restartable); optionally input amplitudes computed with a smaller basis set
- ◆ **Franck-Condon, Herzberg-Teller and FCHT analyses**
- ◆ **Vibronic spectra including electronic circular dichroism (ECD) rotational strengths (HF and DFT)**
- ◆ **Resonance Raman spectra**
- ◆ **Ciofini's excited state charge transfer diagnostic (D_{CT})**
- ◆ **Caricato's EOMCC solvation interaction models**
- ◆ CI-Singles and TD-DFT in solution
- ◆ State-specific excitations and de-excitations in solution
- ◆ **An energy range for excitations can be specified for CIS and TD excitation energies**

Self-Consistent Reaction Field Solvation Models

- ◆ New implementation of the Polarized Continuum Model (PCM) facility for energies, gradients and frequencies
- ◆ Solvent effects on vibrational spectra, NMR, and other properties
- ◆ Solvent effects for ADMP trajectory calcs.
- ◆ Solvent effects for ONIOM calculations
- ◆ Enhanced solvent effects for excited states
- ◆ SMD model for ΔG of solvation
- ◆ Other SCRF solvent models (HF & DFT): Onsager energies, gradients and freqs., Isodensity Surface PCM (I-PCM) energies and Self-Consistent Isodensity Surface PCM (SCI-PCM) energies and gradients

Ease-of-Use Features

- ◆ Automated counterpoise calculations
- ◆ Automated optimization followed by frequency or single point energy
- ◆ Ability to easily add, remove, freeze, differentiate redundant internal coords.
- ◆ Simplified isotope substitution and temperature/pressure specification in the route section
- ◆ Optimizations:
 - * **Retrieve the n th geometry from a checkpoint file**
 - * **Recompute the force constants every n th step of a geometry optimization**
 - * **Reduce the maximum number of allowed steps, including across restarts**
 - * **180° flips detected and suppressed for better visualization**
- ◆ Freezing by fragment for ONIOM optimizations
- ◆ Simplified fragment definitions on molecule specifications
- ◆ Many more restartable job types
- ◆ Atom freezing in optimizations by type, fragment, ONIOM layer and/or residue
- ◆ QST2/QST3 automated transition structure optimizations
- ◆ Saving and reading normal modes
- ◆ **%OldChk Link 0 command specifies read-only checkpoint file for data retrieval**
- ◆ Default.Route file for setting calculation defaults
- ◆ **Enhanced set of equivalent Default.Route directives, Link 0 commands, command line options and environment variables**

Integration with External Programs

- ◆ **NBO 6**
- ◆ COSMO/RS
- ◆ AIMPAC WfnX files
- ◆ **Antechamber**
- ◆ **ACID**
- ◆ Pickett's program
- ◆ **DFTB input files**
- ◆ **General external interface script-based automation, results post-processing, interchanging data/calculation results with other programs, and so on:**
 - * **Interface routines in Fortran, Python and Perl (open source)**
 - * Keyword and **Link 0 command** support

GaussView 6 Features at a Glance

Features new to GaussView 6 are in **blue**; features enhanced in GaussView 6 are in **green**.

Examine Molecular Structures

- ♦ Rotate, translate and zoom in 3D in any display using mouse operations and/or a precision positioning toolbar
- ♦ View numeric value for any structural parameter
- ♦ Use multiple synchronized or independent views of same structure (customizable)
- ♦ Manipulate multiple structures as an ensemble
- ♦ Display formats: wire frame, tubes, ball & stick/bond type, space fill (CPK) style
- ♦ View per-atom labels for element, serial number, NMR shielding (when available)
- ♦ Visualize depth with fog feature
- ♦ Display stereochemistry info
- ♦ Highlight, display or hide atoms based on rich selection capabilities (optionally persistent)

Build/Modify Molecules

- ♦ Convenient palettes for atoms, functional groups, rings, amino acids (central fragment, amino- or carboxyl-terminated) and nucleosides (central fragment, C3'-, C5'-terminated, free forms)
- ♦ Custom fragment libraries
- ♦ Import standard molecule file formats:
 - * PDB, **including ones created by AMBER**. Optionally include/discard waters, apply standard residue bonding on PDB import.
 - * Gaussian input (.gjf and .com), output (.log and .out), checkpoint (.chk and .fchk), cube (.cube), and frequency (.gfrq) files
 - * Sybyl .mol2, .ml2; include/convert .mol2 lone pairs
 - * MDL files: .mol, .rxn, .sdf
 - * Crystallographic Information files: .cif
 - * Optionally include intermediate structures from optimizations, scans, etc.
- ♦ Accurately add hydrogens automatically or manually to an entire molecule or a selection
- ♦ **An advanced open dialog, allowing options to be customized and retained across sessions:**
 - * **Reading intermediate geometries**
 - * **Using the bond table and weak bond inclusion**
 - * **Gaussian input & log file load orders**
 - * **PDB and .mol2 file settings**
 - * **Saving the formatted checkpoint file**
- ♦ Modify bond type/length, bond angles, dihedral angles
- ♦ Rationalize structures with an advanced clean function
- ♦ Recompute bonding on demand
- ♦ Increase **or decrease** symmetry of molecular structure; constrain structure to specific point group
- ♦ Mirror invert structure
- ♦ Invert structure about selected atom
- ♦ Place atom/fragment at centroid of selected atoms
- ♦ Define named groups of atoms via:
 - * Click, marquee & **brush** selection modes
 - * Complex filters combining atom type, number, MM settings, ONIOM layer
 - * Select by PDB residue and/or secondary structure (e.g., helix, chain)
 - * Expand selections by bond or proximity
 - * Use groups for display purposes and in Gaussian input
- ♦ Specify nonstandard isotopes
- ♦ Customize fragment placement behavior
- ♦ **Specify custom bonding parameters**

Graphical Setup for Specific Calculations

Specify input for complex calculations via simple mouse/spreadsheet operations:

- ♦ Build unit cells for polymers, 2D surfaces and crystals (periodic boundary conditions)
 - * Constrain to specific space group symmetry
- ♦ Assign atoms to ONIOM layers by
 - * Direct selection
 - * Bond proximity to specified atom
 - * Absolute distance from specified atom
 - * PDB file residue, secondary structure

- * Complex selection criteria
- ♦ View/specify MM atom types and charges
- ♦ Add/redefine redundant internal coordinates
- ♦ Specify frozen atoms/coordinates during optimizations
- ♦ Set atom equivalences for QST2/QST3 TS optimizations
- ♦ Manipulate MOs: Select, rearrange/reoccupy orbitals for CASSCF, etc.
- ♦ Define fragments for fragment guess/counterpoise calculations
 - * Assign fragment-specific charges & spin multiplicities
- ♦ Include PDB data in molecule specification
- ♦ Select normal modes for frequency calculations
- ♦ Specify atoms for NMR spin-spin coupling
- ♦ **Search for conformations using the GMMX add-on**
- ♦ **Full AMPAC integration if software is installed**

Prepare and Run Gaussian Calculations

- ♦ Create input files via a menu-driven interface:
 - * Select job/method/basis from pop-up menus; related options appear automatically
 - * Supports all major **Gaussian 16 features**
 - * Convenient access to commonly-used general options
 - * **Additional input can be entered**; input sections in imported files are retained
 - * **Preview input file before saving/submitted**
- ♦ Select solvent and specify other parameters for calculations in solution
- ♦ **Specify Link 0 commands**
- ♦ **Specify settings for multiprocessor and cluster/network parallel jobs**
- ♦ Use calculation schemes to set up jobs from templates
- ♦ "Quick launch" Gaussian jobs with a single mouse click
- ♦ Molecule specification created automatically
 - * Optional connectivity section
- ♦ Stream log files in a text-searchable window
- ♦ Monitor/control local Gaussian and utility processes
- ♦ **Integrated, customizable queuing system**
- ♦ Initiate remote jobs via a script
- ♦ Generate job-specific input automatically:
 - * PBC translation vector for periodic structures like polymers and crystals
 - * Orbital alterations
 - * Multiple molecule specifications for QST2/QST3 transition state searches
 - * **Fragment guess and counterpoise per-fragment charge and spin multiplicity**
- ♦ **Apply calculation settings to a group of molecules with one click**
- ♦ **Save/submit identical jobs for a group of molecules in a single step, using unique file names**

Examine & Visualize Gaussian Results

- ♦ **Select which jobs to open from multi-step results files**
- ♦ Show calculation results summary, including basic information, **optimization step data and thermochemical results**
- ♦ **Display results tables for a molecule group**
- ♦ Examine atomic charges: numerical values, color atoms by charge, dipole moment vector
- ♦ **Visualize atomic properties, predicted bond lengths and predicted bond orders**
- ♦ Create surfaces and contours for molecular orbitals, electron density, electrostatic potential, spin density, NMR shielding density
 - * Display formats: 3D solid, translucent or wire mesh; 2D contour
 - * Color surfaces by a separate property
 - * Specify the desired contour plane
 - * Load cubes created by Gaussian; save computed cubes for future reuse; perform operations on cubes
- ♦ Animate normal modes:
 - * Indicate motion via displacement vector, dipole derivative unit vector
 - * Displace structures along normal mode
 - * Select subset of modes for display
 - * Save generated normal modes back to checkpoint file
 - * **Scale frequencies**
 - * **Save animations as MP4 movies, with options for speed, aspect ratio, looping, time delay between frames and frames/loop**

- ◆ Display spectra: IR, Raman, NMR, VCD, ROA, UV-Visible, etc.
 - * **Select Harmonic and/or Anharmonic results**
 - * **Customize plot displays**
 - * **Display multiple data sets on a single spectra plot, with optional conformational averaging**
- ◆ Substitute isotopes in frequency analysis
- ◆ Specify incident light frequency for frequency-dependent calculations
- ◆ **Display results from Gaussian trajectory calculations**
- ◆ **View energy plot of conformational search result set**
- ◆ NMR Results:
 - * Report absolute NMR chemical shifts or relative to reference compound
 - * Export NMR summary data as text
- ◆ Animate structure sequences: geometry optimizations, IRC reaction paths, potential energy surface scans, BOMD and ADMP trajectories
 - * Single play or continuous looping; play in reverse
 - * **Save animations as MP4 movies, with options for speed, aspect ratio and frame & endpoint delays**
 - * Plots of related data are also produced
- ◆ Display 3D surface plots for 2-variable scan calculations
- ◆ Customize plot and spectra displays by zooming, scaling, inverting, etc.
 - * Add molecular properties to plots
 - * **Advanced plot customization; line color, canvas and background color, title, x- and y- axis settings, etc.**
 - * **Mixture Editor for multiple overlaid plots**
- ◆ Save any image to a file (including customizations):
 - * Produce web graphics: JPEG, PNG and other formats
 - * Produce publication quality graphics files and printouts: TIFF, JPEG, vector graphics EPS
- * Create images at arbitrary size and resolution
- * Select full color or high quality grey scale formats
- * **Specify custom colors and/or background**
- ◆ Save plots as images or textual data files
- ◆ Save animations in GIF, MNG, MP4 format or as individual frames
- ◆ **Display PCM solvation cavity as a surface**

Customize GaussView

Set/save preferences for most aspects of GaussView functionality:

- ◆ Control building toolbars individually
- ◆ Colors: per-element, molecule window background, surfaces, transparency
- ◆ Builder operation: atom and fragment join methods, adding hydrogens when needed, automated full or partial clean operations, etc.
- ◆ Gaussian 16 calculation settings
- ◆ **Gaussian job execution methods**
- ◆ Display modes
- ◆ Window placement and visibility
- ◆ Icon sizes
- ◆ File/directory locations
- ◆ **Image capture and printing defaults**
- ◆ **Animation settings and movie defaults**
- ◆ Clean function parameters
- ◆ Charge distribution display defaults
- ◆ **Custom bonding parameters**
- ◆ GaussView Tips facility
- ◆ Windows file extension associations
- ◆ **Dialog-specific help system**



Gaussian, Inc.
 340 Quinnipiac St. Bldg. 40
 Wallingford, CT 06492 USA
 custserv@gaussian.com

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