# 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**), checkpoint (**.chk** and **.fchk**), cube (**.cub**), 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 and 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/submitting**
- 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
- Monitor/control local Gaussian and utility processes
- **Integrated, customizable queuing system**
- Stream log files in a text-searchable window
- 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**

## Examining and Visualizing 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
- **Context sensitive help**

For Further Details & Queries, Contact:

**SCUBE Scientific Software Solutions (P) Ltd,**
**1217, (12th Floor), Hemkunt Chambers,**
**89, Nehru Place, New Delhi - 110019.**
**Phone: 011-41618828/29**
**Email: info@scubeindia.com**
**Telefax: 011-41618828**