

# MedeA *Gaussian GUI*

Expanding the limits of computational chemistry

## At-a-Glance

*MedeA*<sup>®1</sup> *Gaussian GUI* provides a graphical user interface to the quantum chemistry code *Gaussian*. *Gaussian* is the software of reference for the quantum chemist. It includes the widest range of quantum chemical methods, including most of the known semi-empirical, DFT, time-dependent, Hartree-Fock, and post-Hartree-Fock methods, as well as a large library of electronic basis sets.

## Key Benefits

- Saves company R&D budget by speeding up research
- Efficient GUI gives access to *Gaussian*
- Fully integrates in the *MedeA Environment*
- Benefits from all *MedeA* functionalities (High Throughput, etc.)
- Offers the widest range of quantum chemical methods and computed molecular properties
- Offers access to the gold standard of molecular properties from high level quantum chemistry

- Easy preparation and submission of routine calculations through *MedeA's Task and Jobserver*
- Generation of valuable results in the computational, high-throughput, and Big Data oriented environment of *MedeA*
- Access to the results and properties in convenient summary files
- Visualization in the *MedeA* graphical environment, as shown in the animation of normal mode of vibration, molecular orbitals, and electrostatic potential figures
- *Gathering and tabulation of Gaussian* data and properties, using the *MedeA HT-launchpad* to constitute molecular databases
- *Complete access to all \*Gaussian* input directives, to create any specific calculation protocol and property calculation, which are readily accessible in the standalone *Gaussian* software

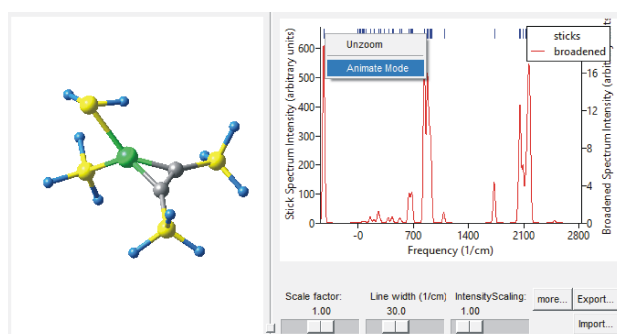


Fig. 1: Animation and visualization of normal modes of vibration calculated with *Gaussian* in *MedeA*<sup>1</sup>

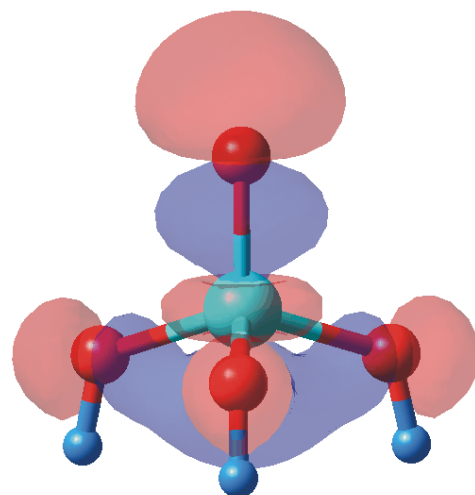


Fig. 2: Visualization of *Gaussian* molecular orbitals calculated with *MedeA*<sup>1</sup>

## Key Features

- Full integration of *GAUSSIAN* into the *MedeA Gaussian GUI*

<sup>1</sup> MedeA and Materials Design are registered trademarks of Materials Design, Inc.

*'Theory attracts practice as the magnet attracts iron.'*

-Carl Friedrich Gauss

## Properties from Gaussian

- Antiferromagnetic coupling
- Atomic charges
- Dipole moment
- Electron affinities
- Electron density
- Electronic circular dichroism (ECD)
- Electrostatic potential
- Electrostatic potential-derived charges
- Electronic transition band shape
- Gibbs free energy of solvation
- High accuracy energies
- Hyperfine coupling constants (anisotropic)
- Hyperfine spectra tensors (including g tensors)
- Ionization potentials
- IR and Raman spectra
- Pre-resonance Raman spectra
- Resonance Raman spectra
- Molecular orbitals
- Multipole moments
- NMR shielding and chemical shifts
- NMR spin-spin coupling constants
- Optical rotations (ORD)
- Polarizabilities and hyperpolarizabilities
- Raman optical activity (ROA)\*
- Thermochemical analysis
- UV/Visible spectra
- Vibration-rotation coupling
- Vibrational circular dichroism (VCD)
- Vibronic (absorption and emission) spectra

The vibrational properties are obtained within the harmonic approximation and include (optionally) anharmonic effects

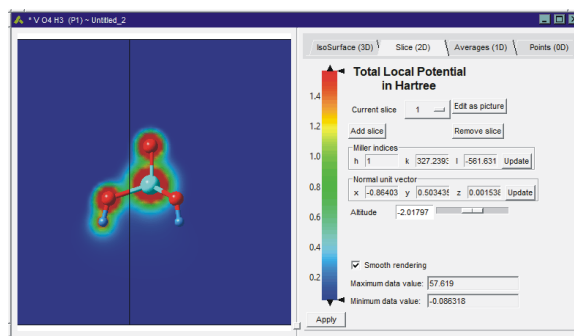


Fig. 3: Visualization of electrostatic potential calculated with Gaussian in Medea<sup>1</sup>

## Required Modules

- *Medea Environment*

## Recommended Modules

- *Medea HT-Launchpad*
- *Medea HT-Descriptor*

## Find Out More

Find out how the *Medea Gaussian GUI* can be employed from our webpage [Materials Design Application Notes](#):

- Energies of stable conformers in heavy alkanes and triglycerides using *Medea*

Learn more about the *Medea Molecular Builder* by watching [How to Build a Complicated Molecule \(MMA\)](#) on the Materials Design Youtube Channel.