MedeA Gaussian GUI

Expanding the limits of computational chemistry

At-a-Glance

MedeA ®[1] *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

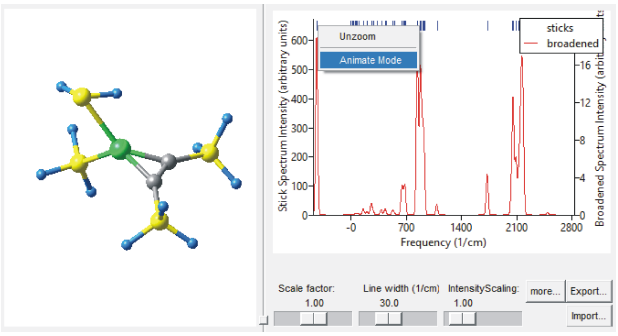

Figure 1: Animation and visualization of normal modes of vibration calculated with Gaussian *in* MedeA[1]

- Easy preparation and submission of routine calculations through *MedeA*'s *Task* and *Jobservers*
- 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

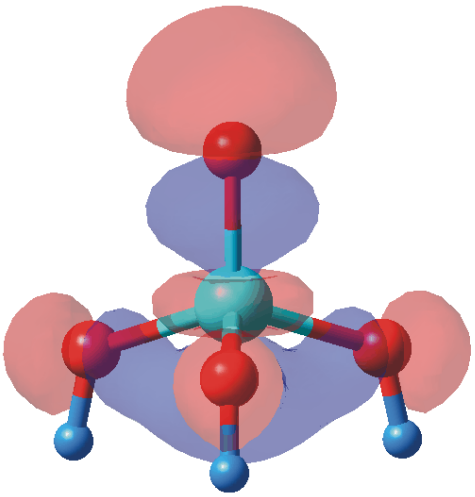

Figure 2: Visualization of Gaussian *molecular orbitals calculated with* MedeA[1]

Key Features

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

'Theory attracts practice as the magnet attracts iron.'

-Carl Friedrich Gauss

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

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

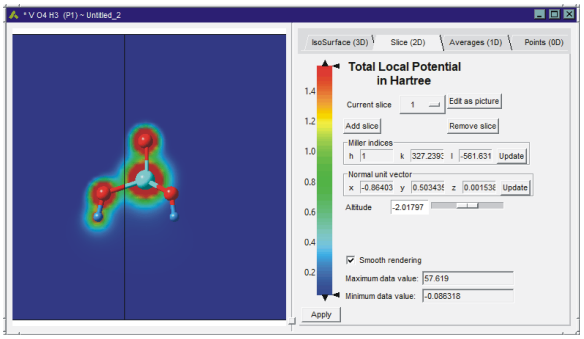

Figure 3: Visualization of electrostatic potential calculated with Gaussian *in* MedeA[1]

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.

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com