BIOVIA MATERIALS STUDIO GAUSSIAN INTERFACE

DATASHEET

The BIOVIA Materials Studio Gaussian Interface® 03 is an intuitive graphical interface for accessing Gaussian's broad range of ab initio modeling methods, including Hartree-Fock, Density Functional Theory (DFT) and sophisticated electron-correlated methods like MP2, CCSD , and G3. The interface helps streamline and enhance your modeling workflows by making it easy for you to set up Gaussian calculations, analyze graphical results, and even exchange molecular structures and properties (including atomic charges and Hessians) between Gaussian's ab initio programs and the force field, semi-empirical, and statistical programs contained within the BIOVIA Materials Studio modeling and simulation environment.

GAUSSIAN—FROM FAST/APPROXIMATE TO ADVANCED/ACCURATE QM METHODS

Researchers working in the chemicals, pharmaceutical, and materials science fields may be tasked with a number of challenging goals, such as developing more efficient catalysts, improving manufacturing processes, or simply gaining a better understanding of molecules, reactions and fundamental processes. Using modeling to explore these challenging problems requires a range of approaches—from fast, approximate methods to highly advanced and accurate techniques.

BIOVIA Materials Studio Gaussian Interface helps you meet your goals by providing a broad range of ab initio capabilities and performing calculations efficiently and reliably, freeing you to choose an approach that provides the most accurate results possible, or one that balances computational cost with accuracy. As stated on BIOVIA Materials Studio Gaussian Interface, Inc.'s website (www.gaussian.com/home.htm), "Starting from the basic laws of quantum mechanics, BIOVIA Materials Studio Gaussian Interface predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types. It can be used to study molecules and reactions under a wide range of conditions, including both stable species and compounds which are difficult or impossible to observe experimentally such as short-lived intermediates and transition structures."

STREAMLINE YOUR WORKFLOWS WITH AN EASY-TO-USE INTERFACE

The BIOVIA Materials Studio Gaussian Interface 03 is part of the BIOVIA Materials Studio software environment, a suite of modeling and simulation tools for studying chemicals and materials, including crystal structure and crystallization processes, polymer properties, catalysis, and structure-activity relationships. All BIOVIA Materials Studio tools are accessible via an intuitive, user-friendly interface that complies with Windows® standards, ensuring that even new users can employ the programs with confidence. For example, the core BIOVIA Materials Studio product—BIOVIA Materials Studio Visualizer—offers a wide range of model building and visualization tools that allow you to rapidly construct models of your systems of interest and easily run advanced QM calculations. After building or reading in a structure, you can control the level of theory, basis set, and convergence options from easy-to-use dialogs, as shown in Figures 1 and 2.

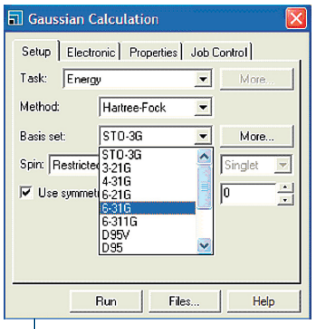

Figure 1: The Setup tab of the BIOVIA Materials Studio User Interface to Gaussian lets you specify a number of input parameters. Here a variety of basis sets are displayed.

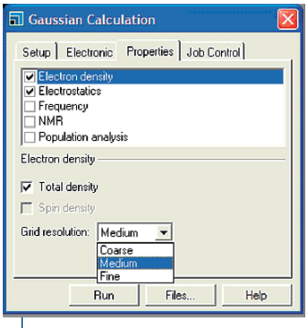

Figure 2: The BIOVIA Materials Studio User Interface to Gaussian makes it easy to request a number of numeric and volumetric properties, such as electron density. This image shows how you can control the resolution used for volumetric rendering.

IMPROVE ANALYSIS AND COLLABORATION WITH QUALITY GRAPHICS

BIOVIA Materials Studio's flexible client-server architecture means that calculations can be run on servers located anywhere on your network. Results are returned to your PC, where they may be displayed and analyzed. You can easily produce high-quality graphics of molecular structures, molecular orbitals, electrostatic potentials, or charge densities, as illustrated in Figure 3. Structures, graphs, and other data produced from the BIOVIA Materials Studio Interface to BIOVIA Materials Studio Gaussian Interface can be instantly exchanged with other PC applications, helping you share results with colleagues or analyze results using spreadsheets and other packages. Gone are the days of transferring files by hand, editing Cartesian coordinates, and running from the command line.

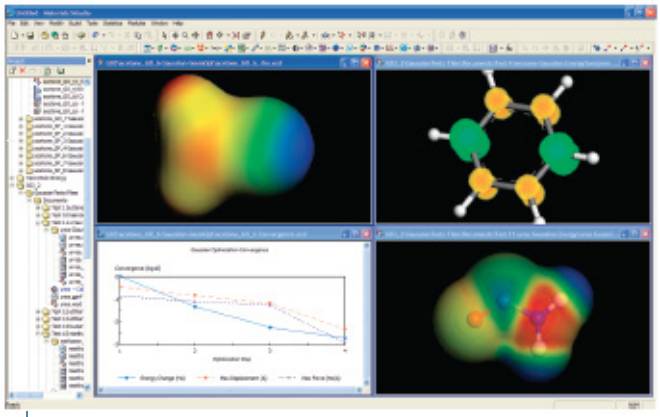

Figure 3: The BIOVIA Materials Studio Gaussian Interface lets you display volumetric properties. Shown here clockwise from the upper left are: 1) charge density of H2CO colored by electrostatic potential; 2) LUMO of benzene; 3) translucent charge density of H2NCO colored by electrostatic potential; 4) convergence of energy and forces for a geometry optimization.

TAKE YOUR MODELING PROJECTS BEYOND QM

As a fully integrated component within the BIOVIA Materials Studio environment, the BIOVIA Materials Studio Gaussian Interface lets you exchange data between Gaussian programs and other BIOVIA Materials Studio modules, making it possible for you to use a single UI to perform sophisticated modeling projects that incorporate force fields, semi-empirical, ab initio, and statistical methods. You can, for example, compute atomic charges with Gaussian, assign them to force fields like BIOVIA Materials Studio COMPASS, and explore the structure of organic crystals with BIOVIA Materials Studio Polymorph Predictor.

A COLLABORATIVE EFFORT— GAUSSIAN AND BIOVIA

The BIOVIA Materials Studio Gaussian Interface represents a collaborative effort by Gaussian and BIOVIA. The powerful and flexible BIOVIA Materials Studio Gaussian Interface 03 program is available from Gaussian, Inc., while BIOVIA distributes the graphical user interface as part of its BIOVIA Materials Studio modeling and simulation environment.

BIOVIA MATERIALS STUDIO GAUSSIAN INTERFACE CAPABILITIES EXPOSED IN THE BIOVIA MATERIALS STUDIO INTERFACE

A number of BIOVIA Materials Studio Gaussian Interface capabilities are available via the BIOVIA Materials Studio User Interface, as detailed below. Please refer to the Gaussian, Inc. website (www.gaussian.com) for a complete list of BIOVIA Materials Studio Gaussian Interface server program capabilities.

Calculation Tasks

- Calculation of total energy
- Geometry minimization

Methods

- DFT (including SVWN, x-Alpha, BLYP, B3LYP, B3PW91, PBEPBE, BB95, BP86)
- MP2, MP4, CID, CISD, QCISD, QCISD(T), CCD, CCSD, CCSD(T),
- BD, BD(T), G1, G2, G3, CBS-4M, CBS-QB3

Basis Sets

- Split valence: STO-3G, 3-21G, 4-31G, 6-21G, 6-31G, 6-311G
- Huzinaga-Dunning: D95 D95V
- Correlation consistent: cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z, cc-pV6Z
- Plus diffuse and polarization functions

Job Control Options

- Specify server machine
- Halt jobs on remote server via BIOVIA Materials Studio Visualizer
- Automatic upload of input files and download of output files

Properties

- Electron density
- Electrostatics
- Vibrational frequency
- NMR Molecular susceptibilities and Spin-spin coupling
- Population analysis

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

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