

# The Leading Molecular Electronic Structure Calculation Software Packages

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Nowadays, molecular systems of tens to hundreds of atoms are routinely studied, thanks to increased computational resources, advanced computing technology and availability of powerful computational software. Computation Chemistry software based on the electronic structure theory plays a very important roles in life science and material science, enabling scientists to perform beyond the capabilities of laboratories and do investigations on the nature and origin of the electronic, optical, and structural properties of a system with high accuracy, but without the need for any experimental input other than the atomic number and mass of the constituent atoms.

There are many software available in this area, and some of them have evolved over the years. This article shares a summary of a few popular software, giving a brief overview of their features and their specialties.

To start, let's take a look at the following wiki page which gives a list of the quantum chemistry and solid state physics software. Most of the software are based on the electronic structure theory:

[http://en.wikipedia.org/wiki/List\\_of\\_quantum\\_chemistry\\_and\\_solid\\_state\\_physics\\_software](http://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid_state_physics_software)

Among all these software, the following are very popular and widely accepted and used by the academic researchers.

**GAUSSIAN:** a computational chemistry software designed to model a broad range of molecular systems under a variety of conditions, performing its computations starting from the basic laws of quantum mechanics. It was initially released in 1970. The current version Gaussian 09 is its 19th versions. Gaussian has implemented almost all the quantum mechanical methods which include Hartree-Fock and post Hartree-Fock method and DFT method. It can be used to calculate the electronic properties, charges, molecular energy, IR, Raman, UV, NMR and other spectroscopic properties of small to media molecules.

Gaussian can also perform Periodic Boundary Conditions (PBC) calculations to model periodic systems in condensed phases: i.e., polymers, surfaces and crystals.

Traditionally, proteins and other large biological molecules have been out of reach of electronic structure methods. However, Gaussian ONIOM method overcomes these limitations. ONIOM first appeared in Gaussian 98, and several significant innovations in Gaussian 03 have made it applicable to much larger molecules.

Gaussian makes use of TCP Linda, a parallel execution environment, to create parallel executables for local area network and the distributed memory multi-processor environments. On a multi-processor, multi-core compute node, Gaussian can run in shared memory parallel mode.

Gaussian's graphical interface, GaussView, provides a powerful facility for building molecular systems and generating their molecule specifications. GaussView can also examine a variety of results graphically, such as electronic properties and spectroscopic properties.

**NWChem:** a general purpose electronic structure program designed for maximum efficiency on massively parallel computers. It can perform density functional, Hartree-Fock, Möller-Plesset, coupled-cluster, configuration interaction, molecular dynamics, and mixed quantum mechanics and molecular mechanics calculations. Geometry optimisations, vibrational frequencies, static one-electron properties, and periodic system modeling are also available.

The NWChem software was developed 15 years ago, and has been shown to scale to thousands of processors (teraflops). It performs well on large systems using MPI and shared memory. NWChem is free for academic researchers.

**GAMESS**: The General Atomic and Molecular Electronic Structure System (GAMESS) is a flexible ab initio electronic structure program. It was developed as early as 1984 and is full-featured and as powerful as Gaussian. Its latest version is able to perform general valence bond, multiconfiguration self-consistent field, Möller-Plesset, coupled-cluster, and configuration interaction calculations. Geometry optimisations, vibrational frequencies, thermodynamic properties, and solution modeling are also available. It performs well on open shell and excited state systems and can model relativistic effects.

Gamess is an open source software and available to academic researchers free of charge.

**CASTEP**: a commercial (and academic) software package which uses density functional theory with a plane wave basis set to calculate electronic properties of solids from first principles. It can be used to simulate a wide range of materials including crystalline solids, such as ceramics, semiconductors, and metals, as well as surfaces, molecules, liquids and amorphous materials. The properties of any material that can be thought of as an assembly of nuclei and electrons can be calculated with the only limitation being the finite speed and memory of the computers being used. It offers simulation capabilities such as accurate prediction of phonon spectra, dielectric constants, and optical properties. In particular, it can predict electronic properties such as band structures and band gaps, Schottky barriers; optical properties such as phonon dispersion curves, polarizability and dielectric constants; or physical properties such as elastic constants.

The commercial CASTEP is integrated with the Accelrys Materials Studio and can be used with the Materials Studio GUI to build up models and display results.

**DMol3**: a unique, accurate, and reliable density functional theory (DFT) quantum mechanical code for research in the chemicals and pharmaceutical industries. It combines computational speed with the accuracy of quantum mechanical methods to predict materials properties both reliably and quickly. It is extremely versatile and can be applied to research problems in the gas phase, solvent, and solid state, in chemistry, materials science, chemical engineering, and solid state physics. It is particularly suited to the study of transition metal compounds and their reactions.

DMol3 comes with the Accelrys Materials Studio, so it is convenient to build the model and display results using Materials Studio's visualiser.

**VASP**: a program package for ab-initio quantum-mechanical molecular dynamics (MD) simulations using either Vanderbilt pseudo-potentials or the projector-augmented wave method with a plane wave basis set. Both techniques allow for a considerable reduction of the necessary number of plane-waves per atom for transition metals and first row elements. Hence we expect VASP to be useful for systems with up to 4,000 valence electrons.

Parallel version of VASP is build using MPI parallel library.