Density Functional Theory (DFT)

- All the capabilities of HyperChem's *Ab Initio* module, e.g. molecular dynamics, vibrations, etc.
- Any combination of seven exchange potentials (Slater, Hartree-Fock, Becke 88, Perdew-Wang 91, Gill 96, PBE 96, HCTH 98) and 7 Correlation Potentials (VWN, Perdew-Zunger 81, Perdew 86, Lee-Yang-Parr, Perdew-Wang 91, PBE 96, HCTH 98).
- Hybrid or Combination Potentials B3-LYP, B3-PW91, EDF1, Becke 97.

Semi-empirical Quantum Mechanics

- HyperChem offers eleven semi-empirical molecular orbital methods, with options for organic and main-group compounds, for transition metal complexes, and for spectral simulation.
- Choose from Extended Hückel, CNDO, INDO, MINDO/3, MNDO, AM1, RM1, PM3, ZINDO/1, ZINDO/S, and TNDO.
- New Typed Neglect of Differential Overlap (TNDO) method that uses semi-empirical parameters assigned to atom types rather than atomic numbers (improved accuracy using ideas from molecular mechanics).
- Applied electric fields (all methods) and magnetic fields (TNDO only).

Molecular Mechanics

- Four force fields provide computationally convenient methods for exploring the stability and dynamics of molecular systems
- Added flexibility of user-defined atom types and parameters.
- Choose from MM+, a general-purpose force field, and three specialized biomolecule force fields: Amber, BIO+(Charmm), and OPLS.
- Convenient inspection and editing of all parameters.

Mixed Mode Calculations

HyperChem allows you to perform quantum calculations on part of a molecular system, such as the solute, while treating the rest of the system classically. This boundary technique is available for semi-empirical methods and, with some limits, for *ab initio* and DFT calculations.

Other Features

Customize and Extend HyperChem with the Chemist's Developer Kit

- Streamline HyperChem's menus. Add new graphical and computational features; create custom menus for specific applications.
- Interface to Visual Basic, C, C++ and FORTRAN programs. Add dialog boxes as well as menu items. For example, you could use HyperChem for visualization of structures and results from non-graphical quantum chemistry programs.
- Link HyperChem procedures to other Windows programs such as MS Word and Excel; direct selected results to these applications for convenient analysis and reporting.
- Use HyperChem's custom script editor to interactively execute script commands or prepare scripts.
- Generate elaborate scripts using the Tcl language and new visual images and dialog boxes with Tk. These standard languages have been extended with over 700 HyperChem script variables and commands.

Interface HyperChem to a Variety of Third-Party Packages such as GAMESS, Gaussian, PQS, Q-Chem and Mopac2007

- Open-source interfaces allow anyone to contribute to and/or extend these interfaces. Interfaces use Visual Studio and C++.
- Interface generates input for third-party package, spawns it and parses its output to return results to HyperChem.
- Follow the simple model to build a graphical interface to any number-crunching package of your own.
- All interfaces initially allow a graphical interface to Single Point calculations for densities and orbitals, Geometry Optimization for display of structure, and vibrational analysis for display and animation of normal modes.

Manuals, Tutorials, and On-line Help

HyperChem includes a full set of electronic manuals in convenient Adobe Acrobat format. These manuals are equivalent to six hardcopy manuals (Getting Started, Reference Manual Vol. 1 and Vol. 2, Modules, Chemist's Developer Kit, and Computational Chemistry). Separate On-line Help is fully integrated into HyperChem including Help within the current Context. A rich set of Video Tutorials is included with HyperChem. Choose from over a hundred tutorials on various topics in molecular modeling and HyperChem. Sit and listen to our CEO describe all the feaures of HyperChem.

Licensing Options

A wide variety of licensing options are available with HyperChem including Hard-Lock (portable dongle - USBt), Soft-Lock (locked to specific machine) and Network Licensing where a license can be used anywhere on a network. Ask us about site licensing for your institution or company.