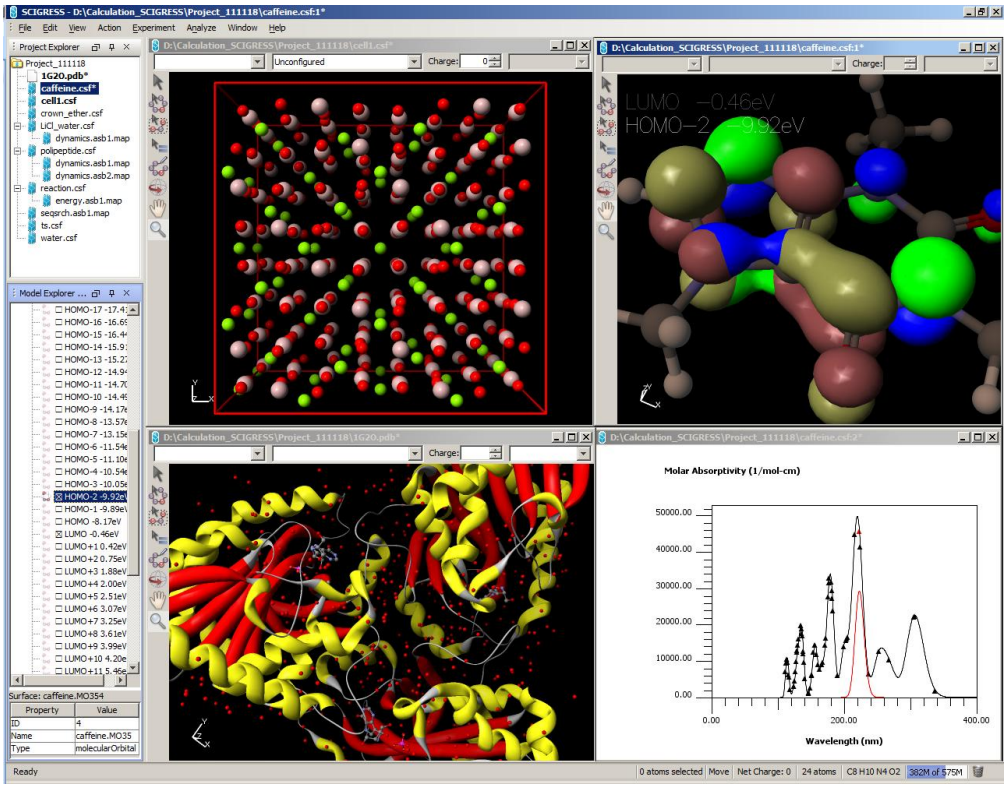
SCIGRESS

SCIGRESS is molecular design modeling software currently available for Microsoft Windows and Linux. A state-of-the-art molecular builder and visualizer enables the researcher to import experiment structures using a variety of industry standard formats, or to build novel structures using a multi-function tool palette. SCIGRESS has the unique ability to apply a wide range of computational models, from molecular mechanics through rigorous quantum electronic structure techniques, to all types of molecular systems, from organic molecules, to inorganics, polymers, materials systems (metals, oxides, ceramics, semiconductors), and whole proteins.

SCIGRESS is a successor of Scigress Explorer (CAChe) and Materials Explorer and integrates both programs into one powerful suite.



Molecular mechanics calculations can be performed on organic and inorganic molecules containing all elements of the periodic table using variety of force fields. Force field parameters can be modified by the user. SCIGRESS includes CONFLEX for automated global minimum searching and systematic generation of low-energy conformers for molecules of any shape, including ring systems.

SCIGRESS provides vast and customizable modeling functions that allow precise control of simulation parameters of advanced molecular dynamics simulation methods that introduce an impressive set of real-world variables and conditions to *in silico* materials experiments. SCIGRESS enables users to set the simulation conditions, such as the number of simulation steps, the ensemble, and potentials, and take complete control of their modeling environment. Users can create their own templates for simulated systems and conditions, as well as set potential assignment rules.

Electronic structure methods in SCIGRESS include Extended Hückel theory (for all elements), ZINDO and MO-S (primarily for UV-visible spectra), and MO-G (previously MOPAC). MO-G, a refinement of MOPAC developed by Fujitsu scientists, covers all main group elements and many metals, with an extensive choice of models including PM6, PM5, AM1, PM3, MINDO/3, and MNDO. It also includes the COSMO solvent model and d-orbitals for transition metals. SCIGRESS quantum chemistry

methods facilitate the study of kinetics and thermodynamics, and the prediction of many physical and chemical properties.

SCIGRESS can transparently run and visualize results from the third party programs: ADF,GAMESS, Gaussian, PHASE, MOPAC2009, and CONFLEX7.

Tools available to the researchers for analyzing molecular structure and properties include the following:

- Reaction mechanism determination via determination of reaction transitions states and evaluation and visualization of intrinsic reaction coordinates.
- Determination of low energy conformations.
- Vibrational analysis including visualization of IR spectra and normal modes of vibration.
- Interactions with radiation including visualization of UV-visible spectra, and identification of molecular orbitals responsible for orbitals electronic transitions.
- 3D-visualization of electronic surfaces including orbitals, electron densities, and electrostatic surfaces.
- Study of phase transitions, expansion, defects, compressibility, tensile strength, adsorption, absorption, thermal conductivity.
- Visualization of experimental crystal and protein structures.

Ready for large systems SCIGRESS can easily interface with large-scale multiprocessor servers to run high performance calculations for very large systems. Highly parallelized compute engines are available for such applications.