MOLCAS

Purpose: Electronic Structure Calculations
Latest version: 8.2
License: ⚠ Must be provided by the user.
Proprietary
Website: *http://www.molcas.org/_ext-link*

MOLCAS is an electronic structure calculations package.

It provides a particular emphasis on multi-configurational methods for highly degenerated ground states. MOLCAS can implement methods for single determinant ground states (SCF, MP2, CC, DFT), but focuses on treating accurately highly degenerate states (excited states, heavy metals, transition states, etc.) through methods such as multi-configurational self-consistent field (MCSCF), complete active space (CASSCF), and including correlation effects via second-order perturbation theory (CASPT2).