OpenMOLCAS

Purpose: Electronic Structure Calculations
Latest version: v21.02
License: Open/Free
Website: *https://gitlab.com/Molcas/OpenMolcas*

OpenMOLCAS (The open version of MOLCAS) is an electronic structure calculations package.

It provides a particular emphasis on multi-configurational methods for highly degenerated ground states. OpenMOLCAS 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).