NewtonX

Purpose: Excited-state molecular dynamics
Latest version: 2b18
Licence: Free of use for non-commercial users
Proprietary _ext-link
Website: *http://newtonx.org/ _ext-link*

NewtonX is a general-purpose program package for excited-state molecular dynamics, including nonadiabatic methods (Trajectory Surface Hopping), and can be used to simulate absorption and emission spectra with the nuclear ensemble approach.

NewtonX modular development allows it to be easily linked to any quantum chemistry package that can provide energy gradients and nonadiabatic couplings