

PSI4NUMPY
PYTHON LIBRARY
BSD-3-Clause

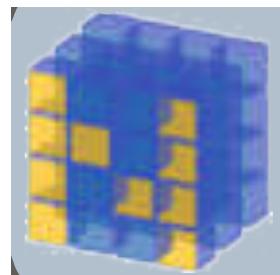
Reference Implementations

RHF SOROHF EP2
EFP/SCF hyperpol
SAPT0(ROHF) MP3
RHF Hessian MD
CCSD(T) EOM-CCSD
FCI CISD
etc.



Tutorials

integrals UHF
DFT VV10 DIIS
CPHF CEPA0 CIS
DF-MP2 OO-MP2
SAPT0
etc.



NumPy
PYTHON LIBRARY
BSD-3-Clause

dependency

