

GQCP::QCModel::RHF
< _Scalar >

+ RHF()
+ RHF()
+ excitationEnergies()
+ spinOrbitalEnergiesBlocked()
+ spinOrbitalEnergiesInterleaved()
+ virtualOrbitalEnergies()
+ occupiedOrbitalEnergies()
+ orbitalEnergies()
+ orbitalEnergy()
+ calculateSingletAStability
Matrix()
and 18 more...
+ calculateElectronicEnergy()
+ calculateError()
+ calculateOrbitalHessianElement()
+ calculateOrbitalHessianTensor()
+ calculateOrbitalHessianFor
ImaginaryResponse()
+ calculateOrthonormalBasis1DM()
+ calculateOrthonormalBasis2DM()
+ calculateScalarBasis1DM()
+ calculateScalarBasis2DM()
+ calculateScalarBasisFock
Matrix()
+ homoIndex()
+ lumoIndex()
+ orbitalSpace()
+ calculatePsocentricMagnetic
Inducibility()
+ calculatePsocentricMagnetic
Inducibility()