

GQCP::QCModel::RHF
< _Scalar >

+ RHF()
+ RHF()
+ calculateOrthonormalBasis1DM()
+ calculateOrthonormalBasis2DM()
+ excitationEnergies()
+ calculateScalarBasis1DM()
+ calculateSingletAStability
Matrix()
+ calculateSingletBStability
Matrix()
+ calculateTripletAStability
Matrix()
+ calculateTripletBStability
Matrix()
and 15 more...
+ calculateElectronicEnergy()
+ calculateError()
+ calculateOrbitalHessianElement()
+ calculateOrbitalHessianTensor()
+ calculateOrthonormalBasis1DM()
+ calculateOrthonormalBasis2DM()
+ calculateScalarBasis1DM()
+ calculateScalarBasisFock
Matrix()
+ homoIndex()
+ lumoIndex()
+ orbitalSpace()