

GQCP::QCModel::UHF
< _Scalar >

+ UHF()
+ UHF()
+ UHF()
+ calculateOrthonormalBasis1DM()
+ calculateOrthonormalBasis2DM()
+ calculateScalarBasis1DM()
+ calculateScalarBasis2DM()
+ calculateMixedSpinConserved
AComponent()
+ calculateMixedSpinConserved
BComponent()
+ calculatePureSpinConserved
AComponent()
and 18 more...
+ calculateElectronicEnergy()
+ calculateError()
+ calculateOrthonormalBasis1DM()
+ calculateOrthonormalBasis2DM()
+ calculateScalarBasis1DM()
+ calculateScalarBasis2DM()
+ calculateScalarBasisDirect
Matrix()
+ calculateScalarBasisExchange
Matrix()
+ calculateScalarBasisFock
Matrix()
+ orbitalSpace()