
GQCP::BaseOrbitalOptimizer
is_converged
convergence_threshold
maximum_number_of_iterations
number_of_iterations
+ BaseOrbitalOptimizer()
+ ~BaseOrbitalOptimizer()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ numberOfIterations()
+ optimize()
GQCP::NewtonOrbitalOptimizer
hessian_modifier
gradient
hessian
+ NewtonOrbitalOptimizer()
+ ~NewtonOrbitalOptimizer()
+ calculateGradientMatrix()
+ calculateHessianTensor()
+ calculateNewFullOrbitalGenerators()
+ prepareOrbitalDerivatives Calculation()
+ calculateNewRotationMatrix()
+ checkForConvergence()
+ prepareConvergenceChecking()
+ calculateGradientVector()
+ calculateHessianMatrix()
+ calculateNewFreeOrbitalGenerators()
+ directionFromIndefiniteHessian()
+ newtonStepIsWellDefined()
GQCP::QCMethodNewtonOrbital Optimizer
D
d
+ ~QCMethodNewtonOrbitalOptimizer()
+ calculate1DM()
+ calculate2DM()
+ prepareDMCalculation()
+ calculateGradientMatrix()
+ calculateHessianTensor()
+ prepareOrbitalDerivatives Calculation()
+ oneDM()
+ twoDM()
+ NewtonOrbitalOptimizer()
GQCP::AP1roGLagrangianNewton OrbitalOptimizer
+ AP1roGLagrangianNewtonOrbital Optimizer()
+ AP1roGLagrangianNewtonOrbital Optimizer()
+ prepareDMCalculation()
+ calculate1DM()
+ calculate2DM()
+ calculateNewFullOrbitalGenerators()
+ electronicEnergy()
+ geminalCoefficients()
+ multipliers()
GQCP::DOCINewtonOrbitalOptimizer < _EigenproblemSolver >
+ DOCINewtonOrbitalOptimizer()
+ calculate1DM()
+ calculate2DM()
+ calculateNewFullOrbitalGenerators()
+ prepareDMCalculation()
+ eigenpair()
+ eigenpairs()
+ makeLinearExpansion()