

ScaLAPACK

Description: A subset of LAPACK routines for parallel calculations.

Site: <http://www.netlib.org/scalapack/>

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Open MPI

Description: Open Source MPI implementation (Version 4)

Site: <https://www.open-mpi.org/community/license.php>

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XCFun

Description: XCFun is a library of DFT exchange-correlation (XC) functionals.

Site: <http://dftlibs.org/xcfun/>

License:

A modified LGPL license that allows us to link ORCA statically with XCFun.

XCFun is copyright 2009-2017 Ulf Ekstrom and contributors.

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Reference:

Ulf Ekström, Lucas Visscher, Radovan Bast, Andreas J. Thorvaldsen and Kenneth Ruud, *Arbitrary-Order Density Functional Response Theory from Automatic Differentiation*, [*Journal of Chemical Theory and Computation* 6, 1971 \(2010\)](#), DOI: [10.1021/ct100117s](https://doi.org/10.1021/ct100117s)

otool_gcp

Description: otool_gcp is used as an external tool that computes an energy correction in order to remove artificial overbinding effects from BSSE.

Site: <https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/gcp/gcp>

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OpenBLAS

Description: OpenBLAS is an optimized BLAS library.

Site: <https://www.openblas.net/>

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Intel® Math Kernel Library (Intel® MKL)

Description: Fastest and most used math library for Intel and compatible processors.

Site: <https://software.intel.com/en-us/intel-mkl>

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Libint

Description: libint is a library of C/C++ functions for efficient evaluation of several kinds of two-body molecular integrals over Gaussian functions and the optimizing compiler that generates a Libint library. Libint version 2 has been integrated into ORCA.

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LibXC

Description: Library of exchange-correlation functionals for density-functional theory (version 5.1).

Site: <https://tddft.org/programs/Libxc/>

Reference:

Susi Lehtola, Conrad Steigemann, Micael J.T. Oliveira, and Miguel A.L. Marques, Recent developments in Libxc - A comprehensive library of functionals for density functional theory, Software X 7, 1 (2018). doi: 10.1016/j.softx.2017.11.002

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* David Strubbe

json

Description: JSON for Modern C++.

Site: <https://github.com/nlohmann/json>

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