MDCI

- Respect MaxCore when building CPCM containers for PTE(S) and PTES.
- UHF-based CCSD producing wrong results with `!CONV`.
- Race condition resulting in wrong results in parallel for PTE(S) and PTES.
- S-diagnostic for canonical RHF and UHF.
- Fixed integral transformation problems.
- Fixed problems with Brückner and orbital optimized UHF CCD.
- Estimate required memory in RI/DLPNO exchange-like integral half-transformation to prevent OOM death.
- Stop calculation if MDCI equations do not converge (same as for SCF).
- Rare pair-pair integral crash.

MP2

- MP2 with ANOs works now.

CASSCF/NEVPT2

- FIX: Custom `EDIAG` failed due to wrong unit conversion - the input energies should now be in Eh.
- FIX: Increased number of states for custom EDIAG (hard-wired).
- FIX: Abort if an unsupported CI solver is requested with TRAH.
- CABSSinglesCorrection is now default in a DLPNO-F12-NEVPT2 (DoCABSSingles=1).
- FIX: MaxIter not properly passed in DLPNO-NEVPT2.
- FIX: QD-NEVPT2 densities not properly used in property calculations.
- FIX: NEVPT2 property calculations now track ground state changes.

MCRPA module

- Removed runtime bottleneck in final CI wave function printing that became an issue for many roots and long CI expansions.

QDPT Module

- `ggauge` was still using `CenterOfNucCharge` for magnetic gauge origin; now uses globally set magnetic origin.
- Other g-tensor fixes to first-order contributions (now consistent with `orca_prop`).
- Issues with QDPT transition densities from ROCIS.

CASSCF QDPT properties

- Corrected indexing of transition densities and ground-state spin densities.
  - Affected properties: EFG tensor, RHO, first-order g-tensor contributions, SOS properties.
- Memory issue in SSC calculation.

QDPT Module Sum-over-states

- Runs now if g-tensor is requested with `DoSOS true` (before, A-tensor had to also be requested).
- SOS g-tensor now gives full agreement with CAS LR (without orbital response) when all roots are included in CAS/MRCI QDPT calculation.
- Corrected general retrieval of transition spin densities.
  - NOTE: SOS is thus only available for methods where transition spin densities are available (now: MRCI, CASSCF, CASSCF+NEVPT2, CASSCF+Custom diagonal energies)

MD Module

- External forces on Colvars are now properly computed (relevant e.g. for thermodynamic integration).
- Many bugfixes (e.g. for the "too many arguments" bug).
- Gradients were not computed for CIS and broken symmetry.

Solvation

- Various options for CPCM: analytic, numeric RI, multipole.
- DRACO keyword not ignored anymore for QM/MM calculations.
- Fix crash for calculations requesting CPCM (bare CPCM / SMD / openCOSMO-RS) if the atomic number of an element in the solute is >= 106.

Dispersion

- Additional `!ATM` alias for the Axilrod-Teller-Muto type three-body-dispersion treatment available via `!ABC`.

EPR

- Crash in `orca_euler` when number of EFG and HFC nuclei differ.

NMR

- ZORA NMR now automatically triggers numeric GIAO 1-el integrals, as in ORCA 5.
- Fixed parallel race condition in DLU-X2C NMR leading to wrong results.
- `Tau=Dobson` default now correctly applied to GIAO calculations.
- Abort for NMR couplings with ZORA (not implemented).
- Fixed hanging of DSO coupling term with X2C when shieldings are also requested.
- Fixed GIAO XC integration for B97-3c with XCFun.

Optimization

- The “big step” fallback should also work if only Cartesian constraints are used.
- Switch off group parallelization if `(Re)CalcHess` is needed.

Relaxed Surface Scan

- Now it allows negative dihedrals on input, improved error report.

DOCKER/SOLVATOR

- Issue when swarming the best structures.
- Fix the chirality of the moment of inertia to avoid creating stereoisomers.
- Wall potential issue when some atoms are very far from the centroid.
- Small fix for solvent dimensions.

Hessian

- Fix for NearIR in `PrintThermoChem` if `InHessName` is different from `BaseName.hess`.
- Fixed issue when writing the IR spectrum multiple times.

X2C

- Disable general contraction for decontracted ANO basis, which led to slowdown.
- CIS/TDDFT gradients with X2C were not picture-change corrected.

Thermochemistry

- D(inf)h point group was not correctly parsed for rotational entropy contribution.

Inertia Tensor

- VPT2 and PAF : Fixed Inertia Tensor calculation.

Rotational Constants

- Minor fixed on unit transformation constants.

Basis sets

- All of SHARK and ORCA now works up to L=10 (except Hessian).

SCF Linear Response

- Fixed issue with initialization of BHP22 solver.

Windows

- Windows-specific crash in `orca_mapspc` fixed.
- Parallel subcalculations in NumCalc (NEB, NumGrad, VPT2, …) now also available on Windows

Property File

- Re-implemented JSON output via the N. Lohmann library (version 3.11.3) to guarantee valid syntax.
- Alleviated memory and timing overhead.
- Respect `%output PropFile=false`/`!NoPropFile` keywords.
- `Quadrupole_Moment`: `EXZ` and `NUCXZ` components held YZ value instead.
- Hessian was stored incorrectly in XTB jobs.
- CIS/TDDFT gradient root was stored incorrectly.
- `Chemical_Shift` components `SPSO`, `SDSO`, and `saniso` were not stored.
- `Calculation_Info` was not stored in some calculations.
- MM, XTB, and ExtOpt jobs now store the geometry and final energy.
- Geometry in JSON output was missing ghost, fragment, and ECP data.

Miscellaneous

- Crash in SOSCF.
- Cleanup leftover files of stability analysis with DFT.
- Atomic fitting density not working with partial general contraction.
- Occasional crash in integral loop.
- Missing PDB file output in QM/MM NEB.
- Prevent crash when reading the nodefile in GOAT, NumFreq, etc.
- Bug in one-sided numerical gradient `TransInvar=true`.
- Restored functionality of `!AIM`.
- Removed leftover temporary files in AUTOCI.
- Restore original irreps if the prediagonalization is skipped in SCF.
- Crash in Hessian for systems with no beta electrons.
- Restored functionality of the `!DoEQ` keyword.
- Opt+NumFreq or Opt+IRC jobs with `!ExtOpt` were stopping after the optimization.
- Print headers for all monitored internals in IRC.
- Fixed HFLD when no pairs are identified.
- Removed RIJCOSX-only restriction for wB97X-3c.
- CP-SCF now aborts if unconverged.
- RI Trafo in CIPSI works now.

- Fixed memory leaks in AO-MP2, QDPT, `orca_2json`, ECPs, ROCIS, LFT, and others.
- Spectrum intensity printing and decomposition in `orca_mapspc` for cases beyond the dipole approximation.
- `orca_vpot`: Fixed ESP calculation when contraction change.

A.1.4 Removed

CASSCF/NEVPT2

- QD-NEVPT2 with Cloiszeaux Hamiltonian (QDType=QD_Cloiszeaux).
- Some options for the handling of reduced density matrices in NEVPT2 (D4Step=core, D4Step=D4PT).

MCRPA module

- If the eigenvalue equations fail to converge, the connection to CASSCF wave function instability is not mentioned anymore. The manual section has also been removed.

A.2 Changes ORCA 6.0.1

A.2.1 Fixed

DFT

- Crash when XCFun functional was overwritten with LibXC.
- Hessian fixed for DFT GGA, NoRI, RKS.
- VV10 Hessian is blocked even if invoked with `CALC_HESS=TRUE` and similar.
- Wrong orbitals for non-self-consistent DFT-NL calculations (wB97M-V, wB97X-V, B97M-V).
- `X_WR2SCAN`:
  - Exchange can now be specified individually in the `%method` block.
  - Fixed crashes when second derivatives are requested.
  - TRAH is now disabled per default when using `X_WR2SCAN`.
  - If second derivatives are requested, will now automatically switch to numerical second derivatives.
  - Added appropriate warnings for the above changes.
- Fixed PBEh-3c gCP parameters for Krypton and Lithium to be consistent with Grimme's stand-alone.
- gCP is now fixed (and extended) for r2SCAN-3c up to Z=103.
- Remove restriction to COSX for wB97X-3c .

TD-DFT

- Ground state gradient for TDDFT calculations with `sgradlist` was wrong.
- `DCORR` 2/3 with `DoSCS` giving wrong results in parallel.
- (D)-Correction not available for full TDDFT.
- Fix for memory estimates for Hessian/TDDFT when running without COSX.
- `FollowIRoot` was not supposed to do anything if the overlap was to small, was still updating.
- Fixed interface to `BHP22` solver in CIS.

MP2

- Crash in conventional U-MP2.
- Parallel crash in RI-MP2 density.
- Crash in (RI-)MP2 gradient with SMD.
- Crash in (RI-)MP2 density with PGC and RIJK.
- MP2+CPCM gradient was wrong.
- Crash in NearIR + B2PLYP.
- Bug with MP2 gradient in property file.

MDCI

- SemiCore was not applied correctly if ECP is present.
- ECP-related crashes.
- Fixed redundant integral generation for specific problems.
- Restored old CITrafos to address reported performance issues.
- Added missing 4th-order doubles term in (T) for RKS reference (already present in UKS-(T), RKS-DLPNO-(T), and UKS-DLPNO-(T) and zero for RHF/UHF reference).
- UHF CIS/STEOM calculation with `UseCISUpdate` is set to `false`.
- RHF STEOM: TD-DFT initial guess.

AutoCI

- Fixed large stack allocation, e.g., in MRCC.
- Fixed runtime behavior for `!Moread Noiter` (falsely reporting “not converged”).
- Fixed `!UseSym` falsely aborting.
- AutoCI gradients: abort at start of a calculation when RI is requested instead of after coupled cluster iterations.

CASSCF/NEVPT2/QD-NEVPT2

- Issue running LR over SA-CASSCF solution.
- Incorrect setting of gauge origin in CASSCF QDPT led to misleading output and in some cases complained about not being able to find densities for the origin evaluation.
- Canonicalize the inactive and virtual spaces of AVAS guesses, to avoid spurious warnings about core orbitals in the following CASSCF calculation.
- AVAS: fixed wrong number of occupied orbitals in case no occupied orbitals should have been selected.
- TRAH-CASSCF: compute generalized Fock matrix which is needed for the CASSCF nuclear gradient.
- Fixed redundant generation of coupling coefficients in the CI guess.
- Fixed ABS/CD spectra in calculation with !UseSym and QD-NEVPT2: The wrong densities were picked for the CASSCF transition moments.
- Fixed ABS/CD when the NEVPT/QD-NEVPT2 ground state differs from CASSCF. Respecitve transition were missing.
- Fixed MCD spectra not using transition densities from QD-NEVPT2 for the flag `DoFullSemiclassical=true`.
- Updated manual: Reported `D4TPre` are updated to the new default value 1e-12. ORCA 5 used `D4TPre=1e-10`.
- Fixed closed-shell case, e.g. CAS(6,3), crashing in NEVPT2.
- Fixed NEVPT2/FIC-NEVPT2 wrong energies or crashing for the Vija class to wrong addressing.
- Fixed ICE densities not stored in density container.

ANISO

- Fixed T and L matrices passed to the single-aniso.
- Fixed wrong number of non-relativistic states passed to single-aniso.

QDPT

- Corrected QDPT transition density for excitations beyond “none”.
- Information added to QDPT AMatrix.
- Issues in QDPT properties in `orca_lft` have been addressed.

QM/MM

- Speed issue for QMMM optimizations.
- Crystal-QMMM and compound crashed.
- Removed leftover files from QMMM-IRC amd QMMM-NEB.

Relativity

- Crash for F12 + X2C/ZORA/DKH.
- Unnecessary abort in AutoCI gradients with X2C/DKH/ZORA.
- Disabled X2C+GIAO+FiniteNuc (not yet implemented).
- 2nd-order PC correction to DKH gDSO now skipped when `fpFWtrafo==false` due to numerical instability.

Solvation

- Disabled analytical gradient and Hessian for XTB calculations requesting CPCMX (not implemented).
- FINAL SINGLE POINT ENERGY for calculations requesting CPCMX was wrong.
- Crash for calculations requesting Freq + CPCM + dummy atoms.
- Crash for QM/QM2 calculations with CPCM requesting excited states.
- Crash for multiple XYZ File Scans for DRACO.
- Crash with CPCM + NoIter + Pal + open-shell.
- Fix for GC and CPCM.

Optimization

- Multi-XYZ optimization crash.
- Random possible break when using GFN-xTB Hessian.
- Random crashes for `RECALC_HESS=TRUE`.
- COPT was saving wrong Cartesian Hessian under certain conditions, would break.
- Maximum number of angles that can be included is fixed + better error message.
- Analytic Hessian as initial Hessian option crashed with IRC.
- Crash in NEB-TS with subsequent Hessian, caused by change of number of parallel processes for NEB (max 32).
- NEB parallelization (will - again - automatically start in parallel, if enough processes are available).

GOAT

- GOAT/DOCKER/SOLVATOR now running on Windows.
- WorkerRandomStart fixed and working as intended.
- `-REACT` and `-EXPLORE` were (by mistake) not included sqrt(NFrag) to number of opts.
- Missing timings for GOAT.

DOCKER

- Abort if all final optimizations fail, was ending normally.
- Do not switch to COPT if constraints are given.

Stability analysis

- Stability analysis + closed-shell systems + post-processing (Hirshfeld, NBO, …).
- `SkipSecondSTAB` was still checking for energy differences between steps. Now will move on regardless.

`orca_2json`

- Exported relativistic integrals were wrong in, HMO and angular momentum were missing.
- Choice of origin corrected.
- Empty `[]` and `[""]` are no longer crashing but disabling the options.
- Invalid property JSON syntax in the following cases:
  - multiple geometries (e.g. optimizations);
  - some jobs with multiple properties of the same kind;
  - CIPSI energies;
  - MDCI EOM energies;
  - XTB jobs;
  - energy extrapolation.

`orca_mapspc`

- XAS/XES broadening functions satisfy FWHM.
- Adjusted .stk files normalization to report band integrals.

Compound

- MORead with same type and number of atoms but different arrangement.
- Bugs in statistical functions.

Miscellaneous

- SOMF(1X) parallel bug in semi-numeric Coulomb.
- Dummy/ghost atoms lead to crash in Hessian (partial fix).
- Fixed bug of Fermi smearing calculations of two-electron systems.
- Hangup in `leanscf_aftermath` when using F12 and ECPs.
- Issues in RIXSSOC, XESSOC spectra in ROCIS have been addressed.
- Issues in computing RI-SSC Integrals have been addressed. This property is now turned on in CASSCF, LFT and MRCI modules.
- Fixed a crash in MD and L-OPT when the input file name was “orca”.
- Default COSX algorithm is set to AUTO everywhere, as originally intended.

- Disable frozen-core approximation when no frozen-core electrons are present.
- `orca_vib` was not able to read hess file from AnFreq run.
- For very small systems restart Hessian could crash.
- Small deviations between the Guess CI Matrix and the Sigma Vector in GS-ROCIS.
- DCD-CAS: Removed left-over files.
- Uncontracted MRCI: Fixed partial general contraction calls in the MRCI integral transformation (crashed before).
- Crash for geometry optimization followed by a vibrational frequency calculation with fixed point group Ci.
- Removal of `posix_memalign`, due to glibc/kernel bug.
- NBO communication fixed.
- Fixes a crash in the integral transformation.
- Crash in `orca_vpot` due to missing prescreening matrix.

A.2.2 Improvements

Output

- Print all orbital energies for `!PrintMOs` and `!LargePrint`.
- Removed redundant warning when using gCP for elements Z > 36 (Kr).
- Added citations for wr2SCAN and DFT-D4 extension.
- Better printing of the spin coupling situation of the states resulting from GS-ROCIS calculations.
- Prepended a counter to irrep labels when printing vibrational frequencies.

`orca_2json`

- Citations added to json output file.
- Absolute path in basename possible.

`orca_mapspc`

- Added support for VCD, XASSOCV and XESSOCV spectrum processing.

Symmetry

- Ensured correctness of gradient cleanup, geometry optimizations with fixed point groups and calculations of vibrational frequencies (for point groups with real irreps using pure Hartree-Fock).
- Ensured correctness of the petite-list algorithm for SCF energy and gradient.

Compound

- Implemented automatic knowledge of basenames.
- Added GOAT interface.

Miscellaneous

- Added ASCII checker to input file.
- Add the possibility to read multi-XYZ files with no '>'.
- QDPT in CASSCF now uses the magnetic origin as defined in `%eprnmr` (if not set, defaults to CenterOfNuCharge for backwards compatibility).
- Reduced disk usage and optimized performance for CASSCF (transition) densities in density container.
- Keep topology in initial IDPP path generation.
- Add CIS Gradient in property file.

A.3 Changes ORCA 6.0.0

A.3.1 SCF and Infrastructure

- Significant improvements to the SOSCF solver to make it more robust, preventing huge steps that break the SCF. Overall improvements on the DIIS solvers.
- Due to the SCF updates, the AutoTRAH is now not so often needed and will start now only from above 50 cycles (`AutoTRAHIter`).
- Improvements to the memory handling of TD-DFT, CP-SCF and the Hessian

A.3.2 Basis sets

- def-TZVP and ma-def-TZVP pseudo-potential basis sets for the actinides (Z = 89, Ac - 103, Lr)
- Lehtola's hydrogenic gaussian basis set family (HGBS) including polarized (HGBSP) and augmented (AHGBS, AHGBSP) variants for all elements up to Oganesson (Z = 118)
- def2-SVPD, def2-TZVPD, def2-TZVPPD, def2-QZVPD, def2-QZVPPD basis sets for lanthanoids
- vDZP Grimme's double-zeta valence basis set
- `!MINIX` now correctly activates the corresponding ECP
- Added user-specified L-limit to AutoAux `AutoAuxLLimit`
- Fixed segfault in dhf-ECP
- Fix for `DelECP` in `%coords`
- Added `ReadFragBasis` keywords read fragment-specific basis sets from a file

A.3.3 Solvation

- New charge correction / compensation algorithm (corrected charges printed in an additional file)
- C-PCM/B scheme for QM/MM calculations
- DDCOSMO and CPCM/X available for XTB calculations and QM/MM calculations
- Generalization of names within all solvation models (C-PCM/SMD/ALPB/DDCOSMO/CPCM-X)
- New discretization scheme for the cavity (C-PCM) based on a constant number of charges per unit of area

A.3.4 DFT

- Allow LibXC functional customization via external parameters
- Simple input keywords added for some LibXC functionals
- Added wB97M(2) functional parameters: must be used with wB97M-V orbitals in a two-step job (compound script available)
- D4 for elements 87 (Fr) - 103 (Lr)
- r2SCAN-3c extension to elements 87 (Fr) - 103 (Lr)
- Simple input keyword for functionals with revised D4 parameters by Grimme (wB97X-D4rev, wB97M-D4rev)
- New hybrid functionals: r2SCANh, r2SCAN0, r2SCAN50, wr2SCAN, wB97X-3c
- New double-hybrid functionals: Pr2SCAN50, Pr2SCAN69, wPr2SCAN50, kPr2SCAN50
- Simple input keywords for 2021 variants of revDSD-PBEP86-D4 and revDOD-PBEP86-D4
- Bugfixes for LibXC combined `*_xc_*` functionals
- Fixed crash for D4 + ghost atoms

A.3.5 Excited states

- Analytical gradient for meta-GGA functionals
- Small bugfix to spin-adapted triplets and NACMEs.
- The FolllowIRoot for excited state optimization uses now a much more robust algorithm.
- New implementation for UHF EOM-CCSD and STEOM-CCSD.
- Core ionization/excitation energies using UHF IP-EOM-CCSD and STEOM-CCSD.

A.3.6 Relativity

- Enabled `NumGrad` with relativistic methods
- Second order DKH picture-change correction of contact density
- Minor fixes in DKH picture-change corrections of magnetic properties
- Picture change corrections are activated automatically

A.3.7 Multiscale

- Reading PDB files for 10k+ atoms with HETATMs now possible
- Enabled correct FlipSpin behavior with QMMM
- More efficient MM Module
- Implemented wall potential

A.3.8 Coupled cluster / DLPNO

- Implemented energy ordering for PNO generation
- Added semicore treatment for DLPNO
- Enable DLPNO-CCSD(T) calculations to run DLPNO-CCSD unrelaxed densities

A.3.9 MP2

- Corrected memory estimates and batching in response and gradient
- Removed the slow and limited analytic (RI-)MP2 Hessian code
- Removed non-default Gamma-in-core option for RI-MP2 response
- Disabled single-precision calculations
- Disabled SemiDirect option in AO-MP2
- Enabled range-separated DHDFT gradients with RIJDX

A.3.10 NEB

- Improved IDPP initial path
- More efficient GFN-xTB runs for NEB

A.3.11 COSX

- Improvements to numerical integration grids, both for DFT and COSX
- Faster grid step
- Improved performance and accuracy in COSX, also for the gradient and Hessian

A.3.12 Properties

- NMR spin-spin coupling:
  - Added `SpinSpinElemPairs` and `SpinSpinAtomPairs` keywords to limit which couplings are computed
  - Reduced the number of CP-SCF perturbations necessary via a stochastic selection
  - DSO term was transposed.
  - Off-diagonal PSO elements had the wrong sign
  - Efficiency improvement: solve SD/FC CP-SCF equations in restricted mode for RHF, instead of always using UHF
- Optimized numeric integration for HFC gauge correction

- Removed `RITRAFO` option for CP-SCF
- Switched to `tau=Dobson` as default handling of the kinetic energy density in meta-GGA magnetic properties with GIAOs

A.3.13 Hessian

- Improvements to the Hessian to avoid accumulation on numerical noise and reduce the number of spurious negative frequencies.

A.3.14 Geometry Optimization

- Several improvements to the geometry optimization, making is much more stable. Complete redesign of the Cartesian optimizer (!COPT), making it quick enough to be used together with faster methods.
- Fallbacks in the geometry optimization in case something fails, e.g. if the internal coordinates are unacceptable.
- Arbitrary spherical, ellipsoidal or box-like wall potentials can be added, which will reflect on the energy and gradients and can be used during geometry optimization.

A.3.15 Miscellaneous

- CHELPG charges that reproduce the ESP together with the molecular dipole moment
- Fixed issues with constraints in multi-step jobs
- Molden output: store ECP info in `[Pseudo]` block, set point charge atomic number to 0, handling of ghost atoms
- Made the `ExtOpt` interface easier to use
- Store energy from NEB and IRC in the XYZ file

APPENDIX

B

PUBLICATIONS RELATED TO ORCA

The generic references for ORCA are:

- Neese, Frank. The ORCA program system. *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, **2012**, 2 (1), 73–78. DOI: http://doi.wiley.com/10.1002/wcms.81.
- Neese, Frank. Software update: the ORCA program system, version 4.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, **2018**, 8 (1), e1327. DOI: http://doi.wiley.com/10.1002/wcms.1327.
- Neese, Frank. Software update: The ORCA program system—Version 5.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, **2022**, 12 (5), e1606. DOI: 10.1002/wcms.1606.
- Neese, Frank. Software Update: The ORCA Program System—Version 6.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, **2025**, 15 (2), e70019. DOI: 10.1002/wcms.70019.
- Neese, Frank; Wennmohs, Frank; Becker, Ute; Riplinger, Christoph. The ORCA quantum chemistry program package. *J. Chem. Phys.*, **2020**, 152 (22), 224108. DOI: https://aip.scitation.org/doi/10.1063/5.0004608.

Please do not only cite the above generic reference, but also cite in addition the original papers that report the development and implementation of the methods you have used in your studies! The following publications describe functionality implemented in . We would highly appreciate if you cite them when you use the program.

B.1 Method development

B.1.1 2025

1. Wittmann, Lukas; Garcia-Ratés, Miquel; Riplinger, Christoph. Analytical First Derivatives of the SCF Energy for the Conductor-like Polarizable Continuum Model with Non-Static Radii. J. Comput. Chem., **2025**. DOI: 10.1002/jcc.70099.
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4. Guo, Yang; Sivalingam, Kantharuban; Chilkuri, Vijay Gopal; Neese, Frank. Approximations of density matrices in N-electron valence state second-order perturbation theory (NEVPT2). III. Large active space calculations with selected configuration interaction reference. *J. Chem. Phys.*, **2025**, 162 (14), 144110. DOI: 10.1063/5.0262473.
5. Helmich-Paris, Benjamin; Kjellgren, Erik Rosendahl; Jensen, Hans Jørgen Aa. Excited-State Methods Based on State-Averaged Long-Range CASSCF Short-Range DFT. under review in Phys. Chem. Chem. Phys., **2025**.
6. de Souza, Bernardo. GOAT: A Global Optimization Algorithm for Molecules and Atomic Clusters. *Angew. Chem. Int. Ed.*, **2025**, 64 (18), e202500393. DOI: 10.1002/anie.202500393.

7. Leyser da Costa Gouveia, Tiago; Maganas, Dimitrios; Neese, Frank. General Spin-Restricted Open-Shell Configuration Interaction Approach: Application to Metal K-Edge X-ray Absorption Spectra of Ferro- and Antiferromagnetically Coupled Dimers. *The Journal of Physical Chemistry A*, **2025**, 129 (1), 330–345. PMID: 39680653. arXiv:https://doi.org/10.1021/acs.jpca.4c05228, DOI: 10.1021/acs.jpca.4c05228.

8. Casanova-Páez, M.; Neese, F. Core-Excited States for Open-Shell Systems in Similarity-Transformed Equation-of-Motion Theory. *J. Chem. Theory Comput.*, **2025**, 21 (3), 1306–1321. DOI: 10.1021/acs.jctc.4c01181.

9. Regni, Gianluca; Baldinelli, Lorenzo; Bistoni, Giovanni. A Quantum Chemical Method for Dissecting London Dispersion Energy into Atomic Building Blocks (In press). **2025**. DOI: 10.1021/acscentsci.5c00356.

10. Colinet, Pauline; Neese, Frank; Helmich-Paris, Benjamin. Improving the Efficiency of Electrostatic Embedding Using the Fast Multipole Method. *J. Comput. Chem.*, **2025**, 46 (1), e27532. DOI: 10.1002/jcc.27532.

11. Neese, Frank; Colinet, Pauline; DeSouza, Bernardo; Helmich-Paris, Benjamin; Wennmohs, Frank; Becker, Ute. The "Bubblepole" (BUPO) Method for Linear-Scaling Coulomb Matrix Construction with or without Density Fitting. *J. Phys. Chem. A*, **2025**, 129 (10), 2618–2637. DOI: 10.1021/acs.jpca.4c07415.

12. Lang, Lucas; Chilkuri, Vijay Gopal; Neese, Frank. Treating Spin–Orbit Coupling and Spin–Spin Coupling in the Framework of the Iterative Configuration Expansion Selected CI method (In press). **2025**. DOI: 10.1021/acs.jctc.5c00463.

B.1.2 2024

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