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# Corrigendum: Coupled cluster theory on modern heterogeneous supercomputers

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## A Corrigendum on

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In the published article, the bibliography file was corrupted. As a consequence there were several inconsistencies within the citation list: titles did not match author lists or journal name or were parsed wrong and added in parts to a citation. Additionally, there were a few references included in the published version of the manuscript that were not a part of the original bibliography. The correct **References** list appears below.

The authors apologize for this error and state that this does not change the scientific conclusions of the article in any way. The original article has been updated.

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## References

- Abyar, F., and Novak, I. (2022). Electronic structure analysis of riboflavin: OVGf and EOM-CCSD study. *Acta A Mol. Biomol. Spectrosc.* 264, 120268. doi:10.1016/j.saa.2021.120268
- Adler, T. B., Werner, H. J., and Frederick, R. (2009). Local explicitly correlated second-order perturbation theory for the accurate treatment of large molecules. *J. Chem. Phys.* 130, 054106. doi:10.1063/1.3040174

- Ali, M. F., and Khan, R. Z. (2012). The study on load balancing strategies in distributed computing system. *Int. J. Comput. Sci. Eng. Surv.* 3, 19–30. doi:10.5121/ijces.2012.3203
- Altman, E., Brown, K. R., Carleo, G., Carr, L. D., Demler, E., Chin, C., et al. (2021). Quantum Simulators: architectures and Opportunities. *PRX Quantum* 2, 017003.
- Altun, A., Izsák, R., and Bistoni, G. (2021). Local energy decomposition of coupled-cluster interaction energies: interpretation, benchmarks, and comparison with symmetry-adapted perturbation theory. *Int. J. Quantum Chem.* 121, e26339. doi:10.1002/qua.26339
- Amos, R. D., and Rice, J. E. (1989). Implementation of analytic derivative methods in quantum chemistry. *Comput. Phys. Rep.* 10, 147–187. doi:10.1016/0167-7977(89)90001-4
- Andrade, X., Strubbe, D., De, G., Larsen, A. H., Oliveira, M. J. T., Alberdi-Rodriguez, J., et al. (2015). Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. *Phys. Chem. Chem. Phys.* 17, 31371–31396. doi:10.1039/c5cp00351b
- Ballesteros, F., Dunivan, S. E., and Lao, K. U. (2021). Coupled cluster benchmarks of large noncovalent complexes: the L7 dataset as well as DNA–ellipticine and buckycatcher–fullerene. *J. Chem. Phys.* 154, 154104. doi:10.1063/5.0042906
- Barnes, A. L., Bykov, D., Lyakh, D. I., and Tjerk, P. (2019). Multilayer divide-expand-consolidate coupled-cluster method: demonstrative calculations of the adsorption energy of carbon dioxide in the Mg-MOF-74 metal–organic framework. *J. Phys. Chem. A* 123, 8734–8743. doi:10.1021/acs.jpca.9b08077
- Bartlett, R. J. (2012). Coupled-cluster theory and its equation-of-motion extensions. *Mol. Sci.* 2, 126–138. doi:10.1002/wcms.76
- Bartlett, R. J., and Shavitt, I. (1977). Comparison of high-order many-body perturbation theory and configuration interaction for H<sub>2</sub>O. *Phys. Lett.* 50, 190–198. doi:10.1016/0009-2614(77)80161-9
- Bartlett, R. J., and Silver, D. M. (1974). Correlation energy in LiH, BH, and HF with many-body perturbation theory using Slater-type atomic orbitals. *Int. J. Quantum Chem.* 8, 271–276. doi:10.1002/qua.560080831
- Battagliano, C., Ballard, G., and Tamara, G. (2018). A practical randomized CP tensor decomposition. *SIAM J. Matrix Analysis Appl.* 39, 876–901. doi:10.1137/17m112303
- Baudin, P., Bykov, D., Liakh, D., Ettenhuber, P., and Kristensen, K. (2017). A local framework for calculating coupled cluster singles and doubles excitation energies (LoFEX-CCSD). *Mol. Phys.* 115, 2135–2144. doi:10.1080/00268976.2017.1290836
- Baudin, P., and Kristensen, K. (2016). LoFEX — a local framework for calculating excitation energies: illustrations using RI-CC2 linear response theory. *J. Chem. Phys.* 144, 224106. doi:10.1063/1.4953360
- Baudin, P., Pawłowski, F., Bykov, D., Liakh, D., Kristensen, K., Olsen, J., et al. (2019). Cluster perturbation theory. III. Perturbation series for coupled cluster singles and doubles excitation energies. *J. Chem. Phys.* 150, 134110. doi:10.1063/1.5046935
- Baumgartner, G., Auer, A., Bernholdt, D. E., Bibireata, A., Choppella, V., Cociorva, D., et al. (2005). Synthesis of high-performance parallel programs for a class of *ab initio* quantum chemistry models. *IEEE* 93, 276–292. doi:10.1109/jproc.2004.840311
- Binkley, J. S., and Pople, J. A. (1975). Møller–Plesset theory for atomic ground state energies. *Int. J. Quantum Chem.* 9, 229–236. doi:10.1002/qua.560090204
- Bistoni, G., Riplinger, C., Minenkov, Y., Cavallo, L., Auer, A. A., and Neese, F. (2017). Treating subvalence correlation effects in domain based pair natural orbital coupled cluster calculations: an out-of-the-box approach. *J. Chem. Theory Comput.* 13, 3220–3227. doi:10.1021/acs.jctc.7b00352
- Boudehane, A., Albera, L., Tenenhaus, A., Le Brusquet, L., and Boyer, R. (2022). Parallelization scheme for canonical polyadic decomposition of large-scale high-order tensors. *Signal Processing* 199, 108610.
- Boys, S. F. (1960). Construction of some molecular orbitals to be approximately invariant for changes from one molecule to another. *Rev. Mod. Phys.* 32, 296–299. doi:10.1103/revmodphys.32.296
- Boys, S. F., and Rajagopal, P. (1966). Quantum calculations: which are accumulative in accuracy, unrestricted in expansion functions. *Econ. Comput.* 2, 1–24.
- Bykov, D., and Kjaergaard, T. (2017). The GPU-enabled divide-expand-consolidate RI-MP2 method (DEC-RI-MP2). *J. Comput. Chem.* 38, 228–237. doi:10.1002/jcc.24678
- Bykov, D., Kristensen, K., and Kjaergaard, T. (2016). The molecular gradient using the divide-expand-consolidate resolution of the identity second-order Møller–Plesset perturbation theory: the DEC-RI-MP2 gradient. *J. Chem. Phys.* 145, 024106. doi:10.1063/1.4956454
- Carroll, J. D., and Chang, J. J. (1970). Analysis of individual differences in multidimensional scaling via an n-way generalization of Eckart–Young decomposition. *Psychometrika*, 35, 283–319.
- Cederbaum, L. S. (2008). Born–Oppenheimer approximation and beyond for time-dependent electronic processes. *J. Chem. Phys.* 128, 124101. doi:10.1063/1.2895043
- Christensen, A. S., Kubar, T., Cui, Q., and Elstner, M. (2016). Semiempirical quantum mechanical methods for noncovalent interactions for chemical and biochemical applications. *Chem. Rev.* 116 (9), 5301–5337. doi:10.1021/acs.chemrev.5b00584
- Christiansen, O., Bak, K. L., Koch, H. S., and Stephan, P. A. (1998). A second-order doubles correction to excitation energies in the random-phase approximation. *Phys. Lett.* 284, 47–55. doi:10.1016/s0009-2614(97)01285-2
- Čížek, J. (1966). On the correlation problem in atomic and molecular systems. Calculation of wavefunction components in Ursell-type expansion using quantum-field theoretical methods. *J. Chem. Phys.* 45, 4256–4266. doi:10.1063/1.1727484
- Collins, J. B., Schleyer, V. R., Binkley, J. S., and Pople, J. A. (1976). Self-consistent molecular orbital methods. XVII. Geometries and binding energies of second-row molecules. A comparison of three basis sets. *J. Chem. Phys.* 64, 5142–5151. doi:10.1063/1.432189
- Combes, J.-M., Duclos, P., and Seiler, R. (1981). The Born–Oppenheimer approximation. *Rigorous At. Mol. Phys.*, 185–213.
- Corzo, H. H., Sehanobish, A., and Kara, O. (2021). Learning full configuration interaction electron correlations with deep learning. *Mach. Learn. Phys. Sci. Neural Inf. Processing Syst.*, 35. doi:10.48550/ARXIV.2106.08138
- Dalgaard, E., and Monkhorst, H. J. (1983). Some aspects of the time-dependent coupled-cluster approach to dynamic response functions. *Phys. Rev. A* 28, 1217–1222. doi:10.1103/physreva.28.1217
- Datta, D., and Gordon, M. S. (2021). A massively parallel implementation of the CCSD(T) method using the resolution-of-the-identity approximation and a hybrid distributed/shared memory parallelization model. *J. Chem. Theory Comput.* 17, 4799–4822. doi:10.1021/acs.jctc.1c00389
- Davidson, E. R. (1972). *Nat. orbitals* 6, 235–266.
- Davidson, E. R., and Feller, D. (1986). Basis set selection for molecular calculations. *Chem. Rev.* 86, 681–696. doi:10.1021/cr00074a002
- Davidson, E. R. (1972). Properties and uses of natural orbitals. *Rev. Mod. Phys.* 44, 451–464. doi:10.1103/revmodphys.44.451
- Diaz-Tinoco, M., Dolgounitcheva, O., Zakrzewski, V. G., and Ortiz, J. V. (2016). Composite electron propagator methods for calculating ionization energies. *J. Chem. Phys.* 144, 224110. doi:10.1063/1.4953666
- Dral, P. O., Wu, X., and Thiel, W. (2019). Semiempirical quantum-chemical methods with orthogonalization and dispersion corrections. *J. Chem. Theory Comput.* 15, 1743–1760. doi:10.1021/acs.jctc.8b01265
- Dunning, T. H., Jr. (1989). Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. *J. Chem. Phys.* 90, 1007–1023. doi:10.1063/1.456153
- Edmiston, C., and Krauss, M. (1965). Configuration-interaction calculation of H<sub>3</sub> and H<sub>2</sub>. *J. Chem. Phys.* 42, 1119–1120. doi:10.1063/1.1696050
- Edmiston, C., and Ruedenberg, K. (1963). Localized atomic and molecular orbitals. *Rev. Mod. Phys.* 35, 457–464. doi:10.1103/revmodphys.35.457
- Elstner, M., Frauenheim, T., Kaxiras, E., Seifert, G., and Suhai, S. (2000). A self-consistent charge density-functional based tight-binding scheme for large biomolecules. *Phys. Status Solidi B* 217, 357–376. doi:10.1002/(sici)1521-3951(200011)217:1<357::aid-ssb357>3.0.co;2-j
- Elstner, M., and Seifert, G. (2014). Density functional tight binding. *Philos. Trans. A Math. Phys. Eng. Sci.* 372, 20120483. doi:10.1098/rsta.2012.0483
- Eriksen, J. J., Baudin, P., Ettenhuber, P., Kristensen, K., Kjaergaard, T., and Jørgensen, P. (2015). Linear-scaling coupled cluster with perturbative triple excitations: The divide-expand-consolidate CCSD (T) model. *J. Chem. Theory Comput.* 11, 2984–2993. doi:10.1021/acs.jctc.5b00086
- Eriksen, J. J., Jørgensen, P., and Gauss, J. (2015). On the convergence of perturbative coupled cluster triples expansions: error cancellations in the CCSD (T) model and the importance of amplitude relaxation. *J. Chem. Phys.* 142, 014102. doi:10.1063/1.4904754
- Eriksen, J. J., Kristensen, K., Kjaergaard, T., Jørgensen, P., and Gauss, J. (2014). A Lagrangian framework for deriving triples and quadruples corrections to the CCSD energy. *J. Chem. Phys.* 140, 064108. doi:10.1063/1.4862501
- Eriksen, J. J., Matthews, D. A., Jørgensen, P., and Gauss, J. (2015). Communication: the performance of non-iterative coupled cluster quadruples models. *J. Chem. Phys.* 143, 041101. doi:10.1063/1.4927247
- Ettenhuber, P., Baudin, P., Kjaergaard, T., Jørgensen, P., and Kristensen, K. (2016). Orbital spaces in the divide-expand-consolidate coupled cluster method. *J. Chem. Phys.* 144 (16), 164116. doi:10.1063/1.4947019
- Ettenhuber, P. (2023). *ScaTeLib - a scalable tensor library*.
- Favier, G., and de Almeida, A. L. (2014). Overview of constrained PARAFAC models. *EURASIP J. Adv. Signal Process.* 142. doi:10.1186/1687-6180-2014-142
- Fedorov, D. G. (2017). The fragment molecular orbital method: theoretical development, implementation in GAMESS, and applications. *WIREs Comput. Mol. Sci.*, 7 (6), e1322. doi:10.1002/wcms.1322
- Fedorov, D. G., and Pham, B. Q. (2023). Multi-level parallelization of quantum-chemical calculations. *J. Chem. Phys.* 158 (16), 164106. doi:10.1063/5.0144917
- Foster, I. (1995). *Designing and building parallel programs: Concepts and tools for parallel software engineering*.

- Friedrich, J., and Dolg, M. (2009). Fully automated incremental evaluation of MP2 and CCSD (T) energies: application to water clusters. *J. Chem. Theory Comput.* 5, 287–294. doi:10.1021/ct800355e
- Friedrich, J., and Hänchen, J. (2013). Incremental CCSD(T)(F12\*)/MP2: A black box method to obtain highly accurate reaction energies. *J. Chem. Theory Comput.* 9, 5381–5394. doi:10.1021/ct4008074
- Frisch, M. J., Pople, J. A., and Binkley, J. S. (1984). Self-consistent molecular orbital methods 25. Supplementary functions for Gaussian basis sets. *J. Chem. Phys.* 80, 3265–3269. doi:10.1063/1.447079
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., et al. (2021). Gaussian development version revision. *J.* 15.
- Fung, V., Zhang, J., Juarez, E., and Sumpter, B. G. (2021). Benchmarking graph neural networks for materials chemistry. *Npj Comput. Mater.* 7 (1), 1–8.
- Gonzalez-Escribano, A., Llanos, D. R., Orden, D., and Palop, B. (2006). Parallelization alternatives and their performance on the convex hull problem. *Appl. Math. Model.* 30, 563–577. doi:10.1016/j.apm.2005.05.022
- Götz, A. W., Williamson, M. J., Xu, D., Poole, D., Le Grand, S., and Walker, R. C. (2012). Routine microsecond molecular dynamics simulations with AMBER on GPUs. 1. Generalized born. *Gen. born J. Chem. Theory Comput.* 8, 1542–1555. doi:10.1021/ct200909j
- Grimme, S., Antony, J., Ehrlich, S., and Krieg, H. (2010). A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* 132, 154104. doi:10.1063/1.3382344
- Gyevi-Nagy, L., Kállay, M., and Nagy, P. R. (2021). Accurate reduced-cost CCSD(T) energies: Parallel implementation, benchmarks, and large-scale applications. *J. Chem. Theory Comput.* 17, 860–878. doi:10.1021/acs.jctc.0c01077
- Gyevi-Nagy, L., Kállay, M., and Nagy, P. R. (2019). Integral-direct and parallel implementation of the CCSD(T) method: algorithmic developments and large-scale applications. *J. Chem. Theory Comput.* 16, 366–384. doi:10.1021/acs.jctc.9b00957
- Hagebaum-Reignier, D., Girardi, R., Carissan, Y., and Humbel, S. (2007). Hückel theory for Lewis structures: hückel–Lewis configuration interaction (HL–CI). *J. Mol. Struct. THEOCHEM.* 817, 99–109. doi:10.1016/j.theochem.2007.04.026
- Haghighatdari, M., and Hachmann, J. (2019). Advances of machine learning in molecular modeling and simulation. *Curr. Opin. Chem. Eng.* 23, 51–57. doi:10.1016/j.coche.2019.02.009
- Hampel, C., and Werner, H. J. (1996). Local treatment of electron correlation in coupled cluster theory. *J. Chem. Phys.* 104, 6286–6297. doi:10.1063/1.471289
- Harris, F. E. (1977). Coupled-cluster method for excitation energies. *Int. J. Quantum Chem.* 12, 403–411. doi:10.1002/qua.560120848
- Hasanein, A. A., and Evans, M. W. (1996). *Computational methods in quantum chemistry*, 2.
- Häser, M. (1993). Møller–Plesset (MP2) perturbation theory for large molecules. *Theor. Chim. Acta* 87, 147–173.
- Hättig, C., Hellweg, A., and Köhn, A. (2006). Distributed memory parallel implementation of energies and gradients for second-order Møller–Plesset perturbation theory with the resolution-of-the-identity approximation. *Phys. Chem. Chem. Phys.* 8, 1159. doi:10.1039/b515355g
- Hättig, C., and Weigend, F. (2000). CC2 excitation energy calculations on large molecules using the resolution of the identity approximation. *J. Chem. Phys.* 113, 5154–5161. doi:10.1063/1.1290013
- Head-Gordon, M. R., Rudolph, J., Oumi, M., and Lee, T. J. (1994). A doubles correction to electronic excited states from configuration interaction in the space of single substitutions. *Chem. Phys. Lett.* 219, 21–29. doi:10.1016/0009-2614(94)00070-0
- Hehre, W. J., Stewart, R. F., and Pople, J. A. (1969). Self-consistent molecular-orbital methods. I. Use of Gaussian expansions of Slater-type atomic orbitals. *J. Chem. Phys.* 51, 2657–2664. doi:10.1063/1.1672392
- Helgaker, T., Coriani, S., Jørgensen, P., Kristensen, K., Olsen, J., and Ruud, K. (2012). Recent advances in wave function-based methods of molecular-property calculations. *Chem. Rev.* 112 (1), 543–631. doi:10.1021/cr2002239
- Helgaker, T., Jørgensen, P., and Olsen, J. (2000). *Molecular electronic-structure theory*.
- Helmich, B., and Hättig, C. (2014). A pair natural orbital based implementation of ADC(2)-x: Perspectives and challenges for response methods for singly and doubly excited states in large molecules. *Comput. Theor. Chem.* 1040, 1041 35–44.
- Herbert, J. M. (2019). Fantasy versus reality in fragment-based quantum chemistry. *J. Chem. Phys.* 151, 170901. doi:10.1063/1.5126216
- Hillers-Bendtsen, A. E., Bykov, D., Barnes, A., Liakh, D., Corzo, H. H., Olsen, J., et al. (2023). Massively parallel GPU enabled third-order cluster perturbation excitation energies for cost-effective large scale excitation energy calculations. *J. Chem. Phys.* 158 (14), 144111. doi:10.1063/5.0142780
- Hillers-Bendtsen, A. E., Høyer, N. M., Kjeldal, F. Ø., Mikkelsen, K. V., Olsen, J., et al. (2022). Cluster perturbation theory. VIII. First order properties for a coupled cluster state. *J. Chem. Phys.* 157, 024108. doi:10.1063/5.0082585
- Hitchcock, F. L. (1927). The expression of a tensor or a polyadic as a sum of products. *J. Math. Phys.* 6, 164–189. doi:10.1002/sapm192761164
- Hoy, E. P., and Mazziotti, D. A. (2015). Positive semidefinite tensor factorizations of the two-electron integral matrix for low-scaling *ab initio* electronic structure. *J. Chem. Phys.* 143, 064103. doi:10.1063/1.4928064
- Høyer, N. M., Kjeldal, F. Ø., Hillers, B., Erbs, A., Mikkelsen, K. V., Olsen, J., et al. (2022). Cluster perturbation theory. VI. Ground-state energy series using the Lagrangian. *J. Chem. Phys.* 157, 024106. doi:10.1063/5.0082583
- Høyvik, I. M., Jansik, B., and Jørgensen, P. (2012). Orbital localization using fourth central moment minimization. *J. Chem. Phys.* 137, 224114. doi:10.1063/1.4769866
- Høyvik, I. M., and Jørgensen, P. (2016). Characterization and generation of local occupied and virtual Hartree–Fock orbitals. *Chem. Rev.* 116, 3306–3327. doi:10.1021/acs.chemrev.5b00492
- Høyvik, I. M., Kristensen, K., Jansik, B., and Jørgensen, P. (2012). The divide-expand-consolidate family of coupled cluster methods: numerical illustrations using second order møller–Plesset perturbation theory. *J. Chem. Phys.* 136, 014105. doi:10.1063/1.3667266
- Høyvik, I. M., Kristensen, K., Kjærgaard, T., and Jørgensen, P. (2014). A perspective on the localizability of Hartree–Fock orbitals. *Theor. Chem. Acc.* 133, 1417. doi:10.1007/s00214-013-1417-x
- Ishikawa, T., and Kuwata, K. (2012). RI-MP2 gradient calculation of large molecules using the fragment molecular orbital method. *J. Phys. Chem. Lett.* 3, 375–379. doi:10.1021/jz201697x
- Jakobsen, S., Kristensen, K., and Jensen, F. (2013). Electrostatic potential of insulin: exploring the limitations of density functional theory and force field methods. *J. Chem. Theory Comput.* 9, 3978–3985. doi:10.1021/ct400452f
- Jansik, B., Høst, S., Kristensen, K., and Jørgensen, P. (2011). Local orbitals by minimizing powers of the orbital variance. *J. Chem. Phys.* 134, 194104. doi:10.1063/1.3590361
- Jha, A., Nottoli, M., Mikhalev, A., Quan, C., and Stamm, B. (2022). Linear scaling computation of forces for the domain-decomposition linear Poisson–Boltzmann method. *J. Chem. Phys.* 158 (10), 104105. doi:10.1063/5.0141025
- Kapuy, E., Csépes, Z., and Kozmutza, C. (1983). Application of the many-body perturbation theory by using localized orbitals. *Int. J. Quantum Chem.* 23, 981–990. doi:10.1002/qua.560230321
- Keith, J. A., Vassilev-Galindo, V., Cheng, B., Chmiela, S., Gastegger, M., Müller, K. R., et al. (2021). Combining machine learning and computational chemistry for predictive insights into chemical systems. *Chem. Rev.* 121, 9816–9872. doi:10.1021/acs.chemrev.1c00107
- Khoromskaia, V., and Khoromskij, B. N. (2015). Tensor numerical methods in quantum chemistry: from Hartree–Fock to excitation energies. *Phys. Chem. Chem. Phys.* 17, 31491–31509. doi:10.1039/c5cp01215e
- Kirtman, B. (1995). Local quantum chemistry: the local space approximation for Møller–Plesset perturbation theory. *Int. J. Quantum Chem.* 55 (2), 103–108. doi:10.1002/qua.560550204
- Kjærgaard, T., Baudin, P., Bykov, D., Eriksen, J. J., Ettenhuber, P., Kristensen, K., et al. (2017). Massively parallel and linear-scaling algorithm for second-order Møller–Plesset perturbation theory applied to the study of supramolecular wires. *Comput. Phys. Commun.* 212, 152–160. doi:10.1016/j.cpc.2016.11.002
- Kjærgaard, T., Baudin, P., Bykov, D., Kristensen, K., and Jørgensen, P. (2017). The divide-expand-consolidate coupled cluster scheme. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* 7 e1319.
- Kjærgaard, T. (2017). The Laplace transformed divide-expand-consolidate resolution of the identity second-order Møller–Plesset perturbation (DEC-LT-RIMP2) theory method. *J. Chem. Phys.* 146, 044103. doi:10.1063/1.4973710
- Kleier, D. A., Halgren, T. A., Hall, J. H., and Lipscomb, W. N. (1974). Localized molecular orbitals for polyatomic molecules. I. A comparison of the Edmiston–Ruedenberg and Boys localization methods. *J. Chem. Phys.* 61, 3905–3919. doi:10.1063/1.1681683
- Kolda, T. G., and Bader, B. W. (2009). Tensor decompositions and applications. *SIAM Rev.* 51 (3), 455–500. doi:10.1137/07070111x
- Krause, C., and Werner, H. J. (2012). Comparison of explicitly correlated local coupled-cluster methods with various choices of virtual orbitals. *Phys. Chem. Chem. Phys.* 14, 7591–7604. doi:10.1039/c2cp40231a
- Krishnan, R. B. J. S., Binkley, J. S., Seeger, R., and Pople, J. A. (1980). Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. *J. Chem. Phys.* 72, 650–654. doi:10.1063/1.438955
- Krishnan, R., and Pople, J. A. (1978). Approximate fourth-order perturbation theory of the electron correlation energy. *Int. J. Quantum Chem.* 14, 91–100. doi:10.1002/qua.560140109
- Kristensen, K., Eriksen, J. J., Matthews, D. A., Olsen, J., and Jørgensen, P. (2016). A view on coupled cluster perturbation theory using a bivariational Lagrangian formulation. *J. Chem. Phys.* 144, 064103. doi:10.1063/1.4941605
- Kristensen, K., Høyvik, I. M., Jansik, B., Jørgensen, P., Kjærgaard, T., Reine, S., et al. (2012). MP2 energy and density for large molecular systems with internal error control



- using the Divide-Expand-Consolidate scheme. *Phys. Chem. Chem. Phys.* 14, 15706–15714. doi:10.1039/c2cp41958h
- Kristensen, K., Jørgensen, P., Jansik, B., Kjærgaard, T., and Reine, S. (2012). Molecular gradient for second-order Møller-Plesset perturbation theory using the divide-expand-consolidate (DEC) scheme. *J. Chem. Phys.* 137, 114102. doi:10.1063/1.4752432
- Kristensen, K., Ziolkowski, M., Jansik, B., Kjærgaard, T., and Jørgensen, P. (2011). A locality analysis of the divide-expand-consolidate coupled cluster amplitude equations. *J. Chem. Theory Comput.* 7, 1677–1694. doi:10.1021/ct200114k
- Kurashige, Y., Yang, J., Chan, G. K. L., and Manby, F. R. (2012). Optimization of orbital-specific virtuals in local Møller-Plesset perturbation theory. *J. Chem. Phys.* 136 (12), 124106. doi:10.1063/1.3696962
- Kutzelnigg, W. (2007). What I like about Hückel theory. *J. Comput. Chem.* 28, 25–34. doi:10.1002/jcc.20470
- Article title Frontiers in neuroscience (2013) Article title Frontiers in neuroscience 30 10127–10134.
- Levine, I. N., Busch, D. H., and Shull, H. (2009). *Quantum chemistry*, 6.
- Li, R. R., Liebenthal, M. D., and De Prince Eugene, A. (2021). Challenges for variational reduced-density-matrix theory with three-particle N-representability conditions. *J. Chem. Phys.* 155, 174110. doi:10.1063/5.0066404
- Liakos, D. G., Sparta, M., Kesharwani, M. K., Martin, J. M. L., and Neese, F. (2015). Exploring the accuracy limits of local pair natural orbital coupled-cluster theory. *J. Chem. Theory Comput.* 11, 1525–1539. doi:10.1021/ct501129s
- Lin, N., Marianetti, C. A., Millis, A. J., and Reichman, D. R. (2011). Dynamical mean-field theory for quantum chemistry. *Phys. Rev. Lett.* 106, 096402. doi:10.1103/physrevlett.106.096402
- Lipparini, F., Stamm, B., Cancès, E., Maday, Y., and Mennucci, B. (2013). Fast domain decomposition algorithm for continuum solvation models: energy and first derivatives. *J. Chem. Theory Comput.* 9, 3637–3648. doi:10.1021/ct400280b
- Liu, W. (2020). Essentials of relativistic quantum chemistry. *J. Chem. Phys.* 152, 180901. doi:10.1063/5.0008432
- Löwdin, P. O. (1958). Correlation problem in many-electron quantum mechanics I. Review of different approaches and discussion of some current ideas. *Adv. Chem. Phys.* 207–322.
- Löwdin, P. O. (1955). Quantum theory of many-particle systems. II. Study of the ordinary Hartree-Fock approximation. *Phys. Rev.* 97, 1490–1508. doi:10.1103/physrev.97.1490
- Löwdin, P. O. (1955). Quantum theory of many-particle systems. I. Physical interpretations by means of density matrices, natural spin-orbitals, and convergence problems in the method of configurational interaction. *Phys. Rev.* 97, 1474–1489. doi:10.1103/physrev.97.1474
- Luo, L., Straatsma, T., Suarez, L. E. A., Broer, R., Bykov, D., et al. (2020). Pre-exascale accelerated application development: The ORNL Summit experience, *IBM J. Res. Dev.* 64, 1–11. doi:10.1147/jrd.2020.2965881
- Lyakh, D. I. (2023). *TAL-SH: Tensor algebra library for shared memory computers*.
- Ma, Y., Li, Z. Y., Chen, X., Ding, B., Li, N., Lu, T., et al. (2023). Machine-learning assisted scheduling optimization and its application in quantum chemical calculations. *J. Comput. Chem.* 44, 1174–1188. doi:10.1002/jcc.27075
- Maslow, A. H. (1966). *The psychology of science: A reconnaissance*.
- Menezes, F., Kats, D., and Werner, H. J. (2016). Local complete active space second-order perturbation theory using pair natural orbitals (PNO-CASPT2). *J. Chem. Phys.* 145, 124115. doi:10.1063/1.4963019
- Mester, D., Nagy, P. R., and Kállay, M. (2019). Reduced-Scaling correlation methods for the excited states of large molecules: implementation and benchmarks for the second-order algebraic-diagrammatic construction approach. *J. Chem. Theory Comput.* 15, 6111–6126. doi:10.1021/acs.jctc.9b00735
- Mitxelena, I., and Piris, M. (2022). Benchmarking GNOF against FCI in challenging systems in one, two, and three dimensions. *J. Chem. Phys.* 156, 214102. doi:10.1063/5.0092611
- Moawad, Y., Vanderbauwhede, W., and Steijl, R. (2022). Investigating hardware acceleration for simulation of CFD quantum circuits. *Front. Mech. Eng.* 8, doi:10.3389/fmech.2022.925637
- Møller, C., and Plesset, M. S. (1934). Note on an approximation treatment for many-electron systems. *Phys. Rev.* 46, 618–622. doi:10.1103/physrev.46.618
- Monari, A., Rivail, J. L., and Assfeld, X. (2013). Theoretical modeling of large molecular systems. Advances in the local self consistent field method for mixed quantum mechanics/molecular mechanics calculations. *Acc. Chem. Res.* 46, 596–603. doi:10.1021/ar300278j
- Nagy, B., and Jensen, F. (2017). *Basis sets in quantum chemistry*, 93–149.
- Nagy, P. R., and Kállay, M. (2019). Approaching the basis set limit of CCSD(T) energies for large molecules with local natural orbital coupled-cluster methods. *J. Chem. Theory Comput.* 15, 5275–5298. doi:10.1021/acs.jctc.9b00511
- Neese, F., Wennmohs, F., and Hansen, A. (2009). Efficient and accurate local approximations to coupled-electron pair approaches: an attempt to revive the pair natural orbital method. *J. Chem. Phys.* 130, 114108. doi:10.1063/1.3086717
- Neese, F., Wennmohs, F., Becker, U., and Riplinger, C. (2020). The ORCA quantum chemistry program package. *J. Chem. Phys.* 152, 224108. doi:10.1063/5.0004608
- Nesbet, R. K. (1955). Configuration interaction in orbital theories. *Proc. R. Soc. Lond. A Math. Phys. Sci.* 230, 312–321.
- Nikodem, A., Matveev, A. V., Soini, T. M., and Rösch, N. (2014). Load balancing by work-stealing in quantum chemistry calculations: application to hybrid density functional methods. *Int. J. Quantum Chem.* 114, 813–822. doi:10.1002/qua.24677
- Nottoli, M., Stamm, B., Scalmani, G., and Lipparini, F. (2019). Quantum calculations in solution of energies, structures, and properties with a domain decomposition polarization continuum model. *J. Chem. Theory Comput.* 15, 6061–6073. doi:10.1021/acs.jctc.9b00640
- Olsen, J., Erbs, A., Kjeldal, F. Ø., Høyer, N. M., Mikkelsen, K. V., et al. (2022). Cluster perturbation theory. VII. The convergence of cluster perturbation expansions. *J. Chem. Phys.* 157, 024107. doi:10.1063/5.0082584
- Olsen, J. M. H., List, N. H., Kristensen, K., and Kongsted, J. (2015). Accuracy of protein embedding potentials: An analysis in terms of electrostatic potentials. *J. Chem. Theory Comput.* 11, 1832–1842. doi:10.1021/acs.jctc.5b00078
- Oseledets, I. V. (2011). Tensor-train decomposition. *SIAM J. Sci. Comput.* 33 (5), 2295–2317. doi:10.1137/090752286
- Ozog, D., Hammond, J. R., Dinan, J., Balaji, P., Shende, S., and Malony, A. (2013). “Inspector-executor load balancing algorithms for block-sparse tensor contractions,” in 2013 42nd International conference on parallel processing, 30–39. doi:10.1109/ICPP.2013.12
- Patil, U., and Shedge, R. (2013). Improved hybrid dynamic load balancing algorithm for distributed environment. *Int. J. Sci. Res. Publ.* 3, 1.
- Paudics, A., Hess, D., Bojtár, M., Bitter, I., Horváth, V., Kállay, M., et al. (2022). A pillarene-based indicator displacement assay for the fluorescence detection of vitamin B1. *Sensors Actuators B Chem.* 369, 132364. doi:10.1016/j.snb.2022.132364
- Pawłowski, F., Olsen, J., and Jørgensen, P. (2019a). Cluster perturbation theory. II. Excitation energies for a coupled cluster target state. *J. Chem. Phys.* 150, 134109. doi:10.1063/1.5053167
- Pawłowski, F., Olsen, J., and Jørgensen, P. (2019b). Cluster perturbation theory. I. Theoretical foundation for a coupled cluster target state and ground-state energies. *J. Chem. Phys.* 150, 134108. doi:10.1063/1.5004037
- Pawłowski, F., Olsen, J., and Jørgensen, P. (2019c). Cluster perturbation theory. IV. Convergence of cluster perturbation series for energies and molecular properties. *J. Chem. Phys.* 150, 134111. doi:10.1063/1.5053622
- Pawłowski, F., Olsen, J., and Jørgensen, P. (2019d). Cluster perturbation theory. V. Theoretical foundation for cluster linear target states. *J. Chem. Phys.* 150, 134112. doi:10.1063/1.5053627
- Phan, A. H., Tichavský, P., and Cichocki, A. (2013). Fast alternating LS algorithms for high order CANDECOMP/PARAFAC tensor factorizations. *IEEE Trans. Signal Process.* 61, 4834–4846. doi:10.1109/tsp.2013.2269903
- Pinski, P., and Neese, F. (2018). Communication: exact analytical derivatives for the domain-based local pair natural orbital MP2 method (DLPNO-MP2). *J. Chem. Phys.* 148, 031101. doi:10.1063/1.5011204
- Pipek, J., and Mezey, P. G. (1989). Pair natural orbitals: a concept for simplifying Hartree-Fock and CI wavefunctions. *J. Chem. Phys.* 90, 4916–4926. doi:10.1063/1.456588
- Pople, J. A. (1999). Nobel lecture: Quantum chemical models. *Mod. Phys.* 71, 1267–1274. doi:10.1103/revmodphys.71.1267
- Pople, J. A., Binkley, J. S., and Seeger, R. (1976). Theoretical models incorporating electron correlation. *Int. J. Quantum Chem.* 10, 1–19. doi:10.1002/qua.560100802
- Pulay, P., and Saebø, S. (1986). Orbital-invariant formulation and second-order gradient evaluation in Møller-Plesset perturbation theory. *Chem. Acc.* 69, 357–368. doi:10.1007/bf00526697
- Pulay, P., and Hamilton, T. P. (1988). UHF natural orbitals for defining and starting MC-SCF calculations. *J. Chem. Phys.* 88, 4926–4933. doi:10.1063/1.454704
- Pulay, P. (1983). Localizability of dynamic electron correlation. *Chem. Phys. Lett.* 100, 151–154. doi:10.1016/0009-2614(83)80703-9
- Pykkö, P. (2012). Relativistic effects in chemistry: more common than you thought. *Annu. Rev. Phys. Chem.* 63, 45–64. doi:10.1146/annurev-physchem-032511-143755
- Qiu, J., Zhao, Z., Wu, B., Vishnu, A., and Song, S. (2017). Enabling scalability-sensitive speculative parallelization for FSM computations. *Proc. Int. Conf. Supercomput.*, 2.
- Qiu, Y., Zhou, G., Zhang, Y., and Cichocki, A. (2021). Canonical polyadic decomposition (CPD) of big tensors with low multilinear rank. *Multimed. Tools Appl.* 80, 22987–23007. doi:10.1007/s11042-020-08711-1
- Raghavachari, K., Trucks, G. W., Pople, J. A., and Head-Gordon, M. (1989). A fifth-order perturbation comparison of electron correlation theories. *Chem. Phys. Lett.* 157 (6), 479–483. doi:10.1016/s0009-2614(89)87395-6
- Riplinger, C., and Neese, F. (2013). An efficient and near linear scaling pair natural orbital based local coupled cluster method. *J. Chem. Phys.* 138, 034106. doi:10.1063/1.4773581

- Riplinger, C., Sandhoefer, B., Hansen, A., and Neese, F. (2013). Natural triple excitations in local coupled cluster calculations with pair natural orbitals. *J. Chem. Phys.* 139, 134101. doi:10.1063/1.4821834
- Rolik, Z., Szegedy, L., Ladjánszki, I., Ladóczy, B., and Kállay, M. (2013). An efficient linear-scaling CCSD (T) method based on local natural orbitals. *J. Chem. Phys.* 139, 094105. doi:10.1063/1.4819401
- Russ, N. J., and Crawford, T. D. (2004). Local correlation in coupled cluster calculations of molecular response properties. *Phys. Lett.* 400, 104–111. doi:10.1016/j.cplett.2004.10.083
- Sæbo, S., and Almlöf, J. (1989). Avoiding the integral storage bottleneck in LCAO calculations of electron correlation. *Chem. Phys. Lett.* 154, 83–89. doi:10.1016/0009-2614(89)87442-1
- Sæbo, S., and Pulay, P. (1985). Local configuration interaction: an efficient approach for larger molecules. *Chem. Phys. Lett.* 113, 13–18. doi:10.1016/0009-2614(85)85003-x
- Sæbo, S., and Pulay, P. (1993). Local treatment of electron correlation. *Annu. Rev. Phys. Chem.* 44, 213–236. doi:10.1146/annurev.pc.44.100193.001241
- Sæbo, S., and Pulay, P. (1988). The local correlation treatment. II. Implementation and tests. *J. Chem. Phys.* 88, 1884–1890. doi:10.1063/1.454111
- Saitow, M., Uemura, K., and Yanai, T. (2022). A local pair-natural orbital-based complete-active space perturbation theory using orthogonal localized virtual molecular orbitals. *J. Chem. Phys.* 157, 084101. doi:10.1063/5.0094777
- Schriber, J. B., and Evangelista, F. A. (2017). Adaptive configuration interaction for computing challenging electronic excited states with tunable accuracy. *J. Chem. Theory Comput.* 13, 5354–5366. doi:10.1021/acs.jctc.7b00725
- Schütz, M., Yang, J., Frederick, R., and Werner, H. J. (2013). The orbital-specific virtual local triples correction: OSV-L (t). *J. Chem. Phys.* 138, 054109. doi:10.1063/1.4789415
- Schwilk, M., Ma, Q., Köppl, C., and Werner, H. J. (2017). Scalable electron correlation methods. 3. Efficient and accurate parallel local coupled cluster with pair natural orbitals (PNO-LCCSD). *J. Chem. Theory Comput.* 13, 3650–3675. doi:10.1021/acs.jctc.7b00554
- Semidalas, E., and Martin, J. M. L. (2022). The MOBH35 metal–organic barrier heights reconsidered: Performance of local-orbital coupled cluster approaches in different static correlation regimes. *J. Chem. Theory Comput.* 18, 883–898. doi:10.1021/acs.jctc.1c01126
- Shang, H., Shen, L., Fan, Y., Xu, Z., Guo, C., Liu, J., et al. (2022). Large-Scale Simulation of Quantum Computational Chemistry on a New Sunway Supercomputer. *SC22: Int. Conf. High Perform. Comput. Netw. Storage Anal.* 1–14. doi:10.1109/SC41404.2022.00019
- Shao, Y., Gan, Z., Epifanovsky, E., Gilbert, A. T. B., Wormit, M., Kussmann, J., et al. (2015). Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* 113, 184–215. doi:10.1080/00268976.2014.952696
- Sharapa, D. I., Genaev, A., Cavallo, L., and Minenkov, Y. (2019). A robust and cost-efficient scheme for accurate conformational energies of organic molecules. *ChemPhysChem* 20, 92–102. doi:10.1002/cphc.201801063
- Sho, S., and Odanaka, S. (2019). Parallel domain decomposition methods for a quantum-corrected drift–diffusion model for MOSFET devices. *Phys. Commun.* 237, 8–16. doi:10.1016/j.cpc.2018.10.029
- Simons, J., and Nichols, J. (1997). *Quantum mechanics in chemistry*.
- Sitkiewicz, S. P., Rodriguez-Mayorga, M., Luis Josep, M., and Matito, E. (2019). Partition of optical properties into orbital contributions. *Phys. Chem. Chem. Phys.* 21, 15380–15391. doi:10.1039/c9cp02662b
- Sparta, M., Retegan, M., Pinski, P., Riplinger, C., Becker, U., and Neese, F. (2017). Multilevel approaches within the local pair natural orbital framework. *J. Chem. Theory Comput.* 13, 3198–3207. doi:10.1021/acs.jctc.7b00260
- Stegeman, A. (2006). Degeneracy in Candecomp/Parafac explained for  $p \times p \times 2$  arrays of rank  $p + 1$  or higher. *Psychometrika* 71, 483–501.
- Stoychev, G. L., Auer, A. A., Gauss, J., and Neese, F. (2021). DLPNO-MP2 second derivatives for the computation of polarizabilities and NMR shieldings. *J. Chem. Phys.* 154, 164110. doi:10.1063/5.0047125
- Su, H. C., Jiang, H., and Zhang, B. (2007). Synchronization on Speculative Parallelization of Many-Particle Collision Simulation. *World Congr. Eng. Comput. Sci.*
- Subotnik, J. E., and Head-Gordon, M. (2005). A local correlation model that yields intrinsically smooth potential-energy surfaces. *J. Chem. Phys.* 123, 064108. doi:10.1063/1.2000252
- Surján, P. R. (1999). “An introduction to the theory of geminals,” in *Correlation and localization*, 63–88.
- Szabo, A., and Ostlund, N. S. (2012). *Modern quantum chemistry: Introduction to advanced electronic structure theory*.
- Szabó, P. B., Csóka, J., Kállay, M., and Nagy, P. R. (2021). Linear-Scaling open-shell MP2 approach Algorithm benchmarks and large-scale applications. *J. Chem. Theory Comput.* 17, 2886–2905. doi:10.1021/acs.jctc.1c00093
- Tew, D. P., Klopper, W., and Helgaker, T. (2007). Electron correlation: the many-body problem at the heart of chemistry. *J. Comput. Chem.* 28, 1307–1320. doi:10.1002/jcc.20581
- Tew, D. P. (2019). Principal domains in local correlation theory. *J. Chem. Theory Comput.* 15, 6597–6606. doi:10.1021/acs.jctc.9b00619
- Thiel, W. (2014). Semiempirical quantum–chemical methods. *Rev. Comput. Mol. Sci.* 4, 145–157. doi:10.1002/wcms.1161
- Titov, A. V., Ufimtsev, I. S., Luehr, N., and Martinez, T. J. (2013). Generating efficient quantum chemistry codes for novel architectures. *J. Chem. Theory Comput.* 9 (1), 213–221. doi:10.1021/ct300321a
- Tucker, L. R. (1966). Some mathematical notes on three-mode factor analysis. *Psychometrika* 31, 279–311. doi:10.1007/BF02289464
- Unke, O., Bogojeski, M., Gastegger, M., Geiger, M., Smidt, T., and Müller, K. R. (2021). E(3)-equivariant prediction of molecular wavefunctions and electronic densities. *Adv. Neural Inf. Process. Syst.* 34 14434–14447.
- Vahtas, O., Almlöf, J., and Feyereisen, M. W. (1993). Integral approximations for LCAO-SCF calculations. *Chem. Phys. Lett.* 213, 514–518. doi:10.1016/0009-2614(93)89151-7
- Valiev, M., Bylaska, E. J., Govind, N., Kowalski, K., Straatsma, T. P., Van Dam, H. J. J., et al. (2010). NWChem: a comprehensive and scalable open-source solution for large scale molecular simulations. *Phys. Commun.* 181, 1477–1489. doi:10.1016/j.cpc.2010.04.018
- Vannieuwenhoven, N., Meerbergen, K., and Vandebril, R. (2015). Computing the gradient in optimization algorithms for the CP decomposition in constant memory through tensor blocking. *SIAM J. Sci. Comput.* 37 (3), C415–C438. doi:10.1137/14097968x
- Wang, B., Yang, K. R., Xu, X., Isegawa, M., Leverentz, H. R., and Truhlar, D. G. (2014). Quantum mechanical fragment methods based on partitioning atoms or partitioning coordinates. *Accounts Chem. Res.* 47, 2731–2738. doi:10.1021/ar500068a
- Wang, H., Neese, C. F., Morong, C. P., Kleshcheva, M., and Oka, T. (2013). High-Resolution near-infrared spectroscopy of and its deuterated isotopologues. *J. Phys. Chem. A* 117 9908–9918.
- Wang, Y. M., Hättig, C., Reine, S., Valeev, E., Kjærgaard, T., and Kristensen, K. (2016). Explicitly correlated second-order Møller-Plesset perturbation theory in a Divide-Expand-Consolidate (DEC) context. *J. Chem. Phys.* 144, 204112. doi:10.1063/1.4951696
- Wang, Y., Ni, Z., Neese, F., Li, W., Guo, Y., and Li, S. (2022). Cluster-in-Molecule method combined with the domain-based local pair natural orbital approach for electron correlation calculations of periodic systems. *J. Chem. Theory Comput.* 18, 6510–6521. doi:10.1021/acs.jctc.2c00412
- Werner, H. J. (1995). “Problem decomposition in quantum chemistry,” in *Domainbased parallelism and problem decomposition methods in computational science and engineering* (SIAM), 239–261. doi:10.1137/1.9781611971507.ch14
- Westermayr, J., Gastegger, M., Schütt, K. T., and Reinhard, J. (2021). Perspective on integrating machine learning into computational chemistry and materials science. *J. Chem. Phys.* 154, 230903. doi:10.1063/5.0047760
- Woolley, R. G., and Sutcliffe, B. T. (1977). Molecular structure and the born–oppenheimer approximation. *Phys. Lett.* 45, 393–398. doi:10.1016/0009-2614(77)80298-4
- Xie, Z. Y., Jiang, H. C., Chen, Q. N., Weng, Z. Y., and Xiang, T. (2009). Second renormalization of tensor-network states. *Phys. Rev. Lett.* 103, 160601. doi:10.1103/physrevlett.103.160601
- Yang, J., Chan, G., Frederick, R., Schütz, M., and Werner, H. J. (2012). The orbital-specific-virtual local coupled cluster singles and doubles method. *J. Chem. Phys.* 136, 144105. doi:10.1063/1.3696963
- Yang, J., Kurashige, Y., ManbyFrederick, R., and Chan, G. K. L. (2011). Tensor factorizations of local second-order Møller–Plesset theory. *J. Chem. Phys.* 134, 044123. doi:10.1063/1.3528935
- Yates, K. (2012). *Hückel molecular orbital theory*.
- Zhang, I. Y., and Grüneis, A. (2019). Coupled cluster theory in materials science. *Front. Mater.* 6. doi:10.3389/fmats.2019.00123
- Zhang, Q., Dwyer, T. J., Tsui, V., Case, D. A., Cho, J., Dervan, P. B., et al. (2004). NMR structure of a cyclic polyamide–DNA complex. *J. Am. Chem. Soc.* 126, 7958–7966. doi:10.1021/ja0373622
- Ziółkowski, M., Jansik, B., Kjærgaard, T., and Jørgensen, P. (2010). Linear scaling coupled cluster method with correlation energy based error control. *J. Chem. Phys.* 133, 014107. doi:10.1063/1.3456535