

BIBLIOGRAPHY

- [1] Zerner, M. C.; Hehenberger, M. *Chem. Phys. Lett.*, **1979**, 62, 550.
- [2] Guest, M. F.; Saunders, V. R. *Mol. Phys.*, **1974**, 28, 819.
- [3] Saunders, V. R.; Hillier, I. H. *Int. J. Quant. Chem.*, **1973**, VII, 699.
- [4] Pulay, P. *Chem. Phys. Lett.*, **1980**, 73, 393.
- [5] Pulay, P. Improved SCF Convergence Acceleration. *J. Comput. Chem.*, **0024**, 3 (4), 556–560. DOI: [10.1002/jcc.540030413](https://doi.org/10.1002/jcc.540030413).
- [6] Kollmar, Christian. The role of energy denominators in self-consistent field (SCF) calculations for open shell systems. *J. Chem. Phys.*, **1996**, 105 (18), 8204–8212. DOI: [10.1063/1.472674](https://doi.org/10.1063/1.472674).
- [7] Kollmar, Christian. Convergence optimization of restricted open-shell self-consistent field calculations. *Int. J. Quant. Chem.*, **1997**, 62 (6), 617–637. DOI: [10.1002/\(SICI\)1097-461X\(1997\)62:6<617::AID-QUA2>3.0.CO;2-K](https://doi.org/10.1002/(SICI)1097-461X(1997)62:6<617::AID-QUA2>3.0.CO;2-K).
- [8] Fischer, T. H.; Almlöf, J. *J. Phys. Chem.*, **1992**, 96, 9768.
- [9] Neese, F. Approximate Second Order Convergence for Spin Unrestricted Wavefunctions. *Chem. Phys. Lett.*, **2000**, 325, 93–98.
- [10] Bacskay, George B. A Quadratically Convergent Hartree–Fock (QC-SCF) Method. Application to Closed Shell Systems. *Chem. Phys.*, **1981**, 61 (3), 385–404. DOI: [10.1016/0301-0104\(81\)85156-7](https://doi.org/10.1016/0301-0104(81)85156-7).
- [11] Sałek, Paweł; Høst, Stinne; Thøgersen, Lea; Jørgensen, Poul; Manninen, Pekka; Olsen, Jeppe; Jansík, Branislav; Reine, Simen; Pawłowski, Filip; Tellgren, Erik; Helgaker, Trygve; Coriani, Sonia. Linear-Scaling Implementation of Molecular Electronic Self-Consistent Field Theory. *J. Chem. Phys.*, **2007**, 126 (11), 114110.
- [12] Høyvik, Ida-Marie; Jansik, Branislav; Jørgensen, Poul. Trust Region Minimization of Orbital Localization Functions. *J. Chem. Theory Comput.*, **2012**, 8 (9), 3137–3146. DOI: [10.1021/ct300473g](https://doi.org/10.1021/ct300473g).
- [13] Helmich-Paris, Benjamin. A Trust-Region Augmented Hessian Implementation for Restricted and Unrestricted Hartree–Fock and Kohn–Sham Methods. *J. Chem. Phys.*, **2021**, 154 (16), 164104. DOI: [10.1063/5.0040798](https://doi.org/10.1063/5.0040798).
- [14] Harding, D. J.; Gruene, P.; Haertelt, M.; Meijer, G.; Fielicke, A.; Hamilton, S. M.; Hopkins, W. S.; Mackenzie, S. R.; Neville, S. P.; Walsh, T. R. Probing the Structures of Gas-Phase Rhodium Cluster Cations by Far-Infrared Spectroscopy. *J. Chem. Phys.*, **2010**, 133 (21), 214304. DOI: [10.1063/1.3509778](https://doi.org/10.1063/1.3509778).
- [15] Assfeld, X.; Rivail, J.-L. Quantum Chemical Computations on Parts of Large Molecules: The Ab Initio Local Self Consistent Field Method. *Chem. Phys. Lett.*, **1996**, 263, 100–106. DOI: [10.1016/S0009-2614\(96\)01165-7](https://doi.org/10.1016/S0009-2614(96)01165-7).
- [16] Pritchard, Benjamin P.; Altarawy, Doaa; Didier, Brett; Gibson, Tara D.; Windus, Theresa L. New Basis Set Exchange: An Open, Up-to-Date Resource for the Molecular Sciences Community. *J. Chem. Inf. Model.*, **2019**, 59 (11), 4814–4820. DOI: [10.1021/acs.jcim.9b00725](https://doi.org/10.1021/acs.jcim.9b00725).
- [17] Zheng, Jingjing; Xu, Xuefei; Truhlar, Donald G. *Theor. Chem. Acc.*, **2010**, 128, 295–305.

- [18] Rappoport, Dmitrij; Furche, Filipp. *J. Chem. Phys.*, **2010**, 133, 134105.
- [19] Rappoport, Dmitrij. Property-optimized Gaussian basis sets for lanthanides. *J. Chem. Phys.*, **2021**, 155, 124102. DOI: 10.1063/5.0065611.
- [20] Weigend, Florian; Baldes, Alexander. Segmented Contracted Basis Sets for One- and Two-Component Dirac–Fock Effective Core Potentials. *J. Chem. Phys.*, **2010**, 133 (17), 174102. DOI: 10.1063/1.3495681.
- [21] Jensen, Frank. Polarization Consistent Basis Sets: Principles. *J. Chem. Phys.*, **2001**, 115 (20), 9113–9125. DOI: 10.1063/1.1413524.
- [22] Jensen, Frank. Polarization Consistent Basis Sets. II. Estimating the Kohn–Sham Basis Set Limit. *J. Chem. Phys.*, **2002**, 116 (16), 7372–7379. DOI: 10.1063/1.1465405.
- [23] Jensen, Frank; Helgaker, Trygve. Polarization Consistent Basis Sets. V. The Elements Si–Cl. *J. Chem. Phys.*, **2004**, 121 (8), 3463–3470. DOI: 10.1063/1.1756866.
- [24] Jensen, Frank. Polarization Consistent Basis Sets. 4: The Elements He, Li, Be, B, Ne, Na, Mg, Al, and Ar. *J. Phys. Chem. A*, **2007**, 111 (44), 11198–11204. DOI: 10.1021/jp068677h.
- [25] Jensen, Frank. Polarization Consistent Basis Sets. VII. The Elements K, Ca, Ga, Ge, As, Se, Br, and Kr. *J. Chem. Phys.*, **2012**, 136 (11), 114107. DOI: 10.1063/1.3690460.
- [26] Jensen, Frank. Unifying General and Segmented Contracted Basis Sets: Segmented Polarization Consistent Basis Sets. *J. Chem. Theory Comput.*, **2014**, 10 (3), 1074–1085. DOI: 10.1021/ct401026a.
- [27] Jensen, Frank. Segmented Contracted Basis Sets Optimized for Nuclear Magnetic Shielding. *J. Chem. Theory Comput.*, **2015**, 11 (1), 132–138. DOI: 10.1021/ct5009526.
- [28] Lehtola, Susi. Polarized Gaussian Basis Sets from One-Electron Ions. *J. Chem. Phys.*, **2020**, 152 (13), 134108. DOI: 10.1063/1.5144964.
- [29] Yamamoto, Hironori; Matsuoka, Osamu. Accurately Energy-Optimized Gaussian Basis Sets for Hydrogen 1s through 5g Orbitals. *Bulletin of the University of Electro-Communications*, **1992**, 5, 23–34. In Japanese. Citation at <https://ci.nii.ac.jp/naid/40004737908/en/>.
- [30] Noro, Takeshi; Sekiya, Masahiro; Koga, Toshikatsu. Correlating Basis Sets for the H Atom and the Alkali-Metal Atoms from Li to Rb. *Theor. Chem. Acc.*, **2003**, 109, 85–90. DOI: 10.1007/s00214-002-0425-z.
- [31] Noro, Takeshi; Sekiya, Masahiro; Koga, Toshikatsu. Segmented Contracted Basis Sets for Atoms H through Xe: Sapporo-(DK)-nZP Sets (n = D, T, Q). *Theor. Chem. Acc.*, **2012**, 131, 1124. DOI: 10.1007/s00214-012-1124-z.
- [32] Partridge, Harry. Near Hartree–Fock Quality GTO Basis Sets for the Second-Row Atoms. *J. Chem. Phys.*, **1987**, 87 (11), 6643–6647. DOI: 10.1063/1.453450.
- [33] Partridge, Harry. Near Hartree–Fock Quality GTO Basis Sets for the First- and Third-Row Atoms. *J. Chem. Phys.*, **1989**, 90 (2), 1043–1047. DOI: 10.1063/1.456157.
- [34] Pacios, Luis Fernandez; Christiansen, Peter A. Ab initio relativistic effective potentials with spin-orbit operators. I. Li through Ar. *J. Chem. Phys.*, **1985**, 82 (6), 2664–2671. DOI: 10.1063/1.448263.
- [35] Hurley, M. M.; Pacios, Luis Fernandez; Christiansen, P. A.; Ross, R. B.; Ermler, W. C. Ab initio relativistic effective potentials with spin-orbit operators. II. K through Kr. *J. Chem. Phys.*, **1986**, 84 (12), 6840–6853. DOI: 10.1063/1.450689.
- [36] LaJohn, L. A.; Christiansen, P. A.; Ross, R. B.; Atashroo, T.; Ermler, W. C. Ab initio relativistic effective potentials with spin-orbit operators. III. Rb through Xe. *J. Chem. Phys.*, **1987**, 87 (5), 2812–2824. DOI: 10.1063/1.453069.
- [37] Ross, R. B.; Powers, J. M.; Atashroo, T.; Ermler, W. C.; LaJohn, L. A.; Christiansen, P. A. Ab initio relativistic effective potentials with spin-orbit operators. IV. Cs through Rn. *J. Chem. Phys.*, **1990**, 93 (9), 6654–6670. DOI: 10.1063/1.458934.
- [38] Ross, R. B.; Gayen, Sanjukta; Ermler, W. C. Ab initio relativistic effective potentials with spin-orbit operators. V. Ce through Lu. *J. Chem. Phys.*, **1994**, 100 (11), 8145–8155. DOI: 10.1063/1.466809.
- [39] Ermler, W. C.; Ross, R. B.; Christiansen, P. A. Ab initio relativistic effective potentials with spin-orbit operators. VI. Fr through Pu. *Int. J. Quantum Chem.*, **1991**, 40 (6), 829–846. DOI: 10.1002/qua.560400611.

- [40] Nash, Clinton S.; Bursten, Bruce E.; Ermiler, Walter C. Ab initio relativistic effective potentials with spin-orbit operators. VII. Am through element 118. *J. Chem. Phys.*, **1997**, 106 (12), 5133–5142. DOI: [10.1063/1.473992](https://doi.org/10.1063/1.473992).
- [41] Hay, P. Jeffrey; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for the transition metal atoms Sc to Hg. *J. Chem. Phys.*, **1985**, 82 (1), 270–283. DOI: [10.1063/1.448799](https://doi.org/10.1063/1.448799).
- [42] Wadt, W. R.; Hay, P. Jeffrey. Ab initio effective core potentials for molecular calculations. Potentials for main group elements Na to Bi. *J. Chem. Phys.*, **1985**, 82 (1), 284–298. DOI: [10.1063/1.448800](https://doi.org/10.1063/1.448800).
- [43] Hay, P. Jeffrey; Wadt, W. R. Ab initio effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals. *J. Chem. Phys.*, **1985**, 82 (1), 299–310. DOI: [10.1063/1.448975](https://doi.org/10.1063/1.448975).
- [44] Ehlers, Andreas W.; Böhme, Mechthild; Dapprich, Stefan; Gobbi, Alberto; Höllwarth, Andreas; Jonas, Volker; Köhler, Karl Friedrich; Stegmann, Rainer; Veldkamp, Andre; Frenking, Gernot. A Set of f-Polarization Functions for Pseudo-Potential Basis Sets of the Transition Metals Sc–Cu, Y–Ag and La–Au. *Chem. Phys. Lett.*, **1993**, 208 (1-2), 111–114. DOI: [10.1016/0009-2614\(93\)80086-5](https://doi.org/10.1016/0009-2614(93)80086-5).
- [45] Check, Catherine E.; Faust, Timothy O.; Bailey, John M.; Wright, Brian J.; Gilbert, Thomas M.; Sunderlin, Lee S. Addition of Polarization and Diffuse Functions to the LANL2DZ Basis Set for P-Block Elements. *J. Phys. Chem. A*, **2001**, 105 (34), 8111–8116. DOI: [10.1021/jp011945l](https://doi.org/10.1021/jp011945l).
- [46] Roy, Lindsay E.; Hay, P. Jeffrey; Martin, Richard L. Revised Basis Sets for the LANL Effective Core Potentials. *J. Chem. Theory Comput.*, **2008**, 4 (7), 1029–1031. DOI: [10.1021/ct8000409](https://doi.org/10.1021/ct8000409).
- [47] Papajak, Ewa; Truhlar, Donald G. Convergent Partially Augmented Basis Sets for Post-Hartree-Fock Calculations of Molecular Properties and Reaction Barrier Heights. *J. Chem. Theory Comput.*, **2011**, 7 (1), 10–18. DOI: [10.1021/ct1005533](https://doi.org/10.1021/ct1005533).
- [48] Neese, F.; Valeev, E. F. Revisiting the Atomic Natural Orbital Approach for Basis Sets: Robust Systematic Basis Sets for Explicitly Correlated and Conventional Correlated ab initio Methods. *J. Chem. Theory Comput.*, **2011**, 7, 33–43.
- [49] Müller, Marcel; Hansen, Andreas; Grimme, Stefan. ω B97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double- ζ basis set. *J. Chem. Phys.*, **2023**, 158 (1), 014103. DOI: [10.1063/5.0133026](https://doi.org/10.1063/5.0133026).
- [50] Pantazis, D. A.; Chen, X.-Y.; Landis, C. R.; Neese, F. *J. Chem. Theory Comput.*, **2008**, 4, 908–919.
- [51] Bühl, M.; Reimann, C.; Pantazis, D. A.; Bredow, T.; Neese, F. Geometries of Third-Row Transition-Metal Complexes from Density-Functional Theory. *J. Chem. Theory Comput.*, **2008**, 4, 1449–1459. DOI: [10.1021/ct800172j](https://doi.org/10.1021/ct800172j).
- [52] Pantazis, D. A.; Neese, F. *J. Chem. Theory Comput.*, **2009**, 5, 2229–2238.
- [53] Pantazis, D. A.; Neese, F. *J. Chem. Theory Comput.*, **2011**, 7, 677–684.
- [54] Pantazis, D. A.; Neese, F. *Theor. Chem. Acc.*, **2012**, 131, 1292.
- [55] Rolfes, Julian D.; Neese, Frank; Pantazis, Dimitrios A. All-Electron Scalar Relativistic Basis Sets for the Elements Rb–Xe. *J. Comput. Chem.*, **2020**, 41, 1842–1849. DOI: [10.1002/jcc.26355](https://doi.org/10.1002/jcc.26355).
- [56] Aravena, D.; Neese, F.; Pantazis, Dimitrios A. Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. *J. Chem. Theory Comput.*, **2016**, 12, 1148–1156. DOI: [10.1021/acs.jctc.5b01048](https://doi.org/10.1021/acs.jctc.5b01048).
- [57] Pollak, Patrik; Weigend, Florian. Segmented Contracted Error-Consistent Basis Sets of Double- and Triple- ζ Valence Quality for One- and Two-Component Relativistic All-Electron Calculations. *J. Chem. Theory Comput.*, **2017**, 13 (8), 3696–3705. DOI: [10.1021/acs.jctc.7b00593](https://doi.org/10.1021/acs.jctc.7b00593).
- [58] Franzke, Yannick J.; Treß, Robert; Pazdera, Tobias M.; Weigend, Florian. Error-Consistent Segmented Contracted All-Electron Relativistic Basis Sets of Double- and Triple-Zeta Quality for NMR Shielding Constants. *Phys. Chem. Chem. Phys.*, **2019**, 21 (30), 16658–16664. DOI: [10.1039/C9CP02382H](https://doi.org/10.1039/C9CP02382H).
- [59] Stoychev, Georgi L.; Auer, Alexander A.; Neese, Frank. Automatic Generation of Auxiliary Basis Sets. *J. Chem. Theory Comput.*, **2017**, 13 (2), 554. DOI: [10.1021/acs.jctc.6b01041](https://doi.org/10.1021/acs.jctc.6b01041).
- [60] Fuentealba, P.; Preuss, H.; Stoll, H.; von Szentpaly, L. *Chem. Phys. Lett.*, **1982**, 89, 418–422.

- [61] von Szentpaly, L.; Fuentealba, P.; Preuss, H.; Stoll, H. *Chem. Phys. Lett.*, **1982**, 93, 555–559.
- [62] Fuentealba, P.; Stoll, H.; von Szentpaly, L.; Schwerdtfeger, P.; Preuss, H. *J. Phys. B: At. Mol. Opt. Phys.*, **1983**, 16, L323.
- [63] Stoll, H.; P. Fuentealba, P. Schwerdtfeger; Flad, J.; von Szentpaly, L.; Preuss, H. *J. Chem. Phys.*, **1984**, 81, 2732–2736.
- [64] Fuentealba, P.; von Szentpaly, L.; Preuss, H.; Stoll, H. *J. Phys. B: At. Mol. Opt. Phys.*, **1985**, 18, 1287.
- [65] Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. *J. Chem. Phys.*, **1987**, 86, 866–872.
- [66] Igel-Mann, G.; Stoll, H.; Preuss, H. Pseudopotentials for Main Group Elements (IIIA through VIIA). *Mol. Phys.*, **1988**, 65 (6), 1321–1328. DOI: [10.1080/00268978800101811](https://doi.org/10.1080/00268978800101811).
- [67] Dolg, M.; Stoll, H.; Preuss, H. *J. Chem. Phys.*, **1989**, 90, 1730–1734.
- [68] Schwerdtfeger, P.; Dolg, M.; Schwarz, W. H. E.; Bowmaker, G. A.; Boyd, P. D. W. *J. Chem. Phys.*, **1989**, 91, 1762–1774.
- [69] Dolg, M.; Stoll, H.; Savin, A.; Preuss, H. *Theor. Chim. Acta*, **1989**, 75, 173–194.
- [70] Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuss, H. Energy-Adjusted *ab initio* Pseudopotentials for the Second and Third Row Transition Elements. *Theor. Chim. Acta*, **1990**, 77, 123–141. DOI: [10.1007/BF01114537](https://doi.org/10.1007/BF01114537).
- [71] Kaupp, Martin; Schleyer, Paul v. R.; Stoll, Hermann; Preuss, Horst. Pseudopotential Approaches to Ca, Sr, and Ba Hydrides. Why Are Some Alkaline-Earth MX₂ Compounds Bent? *J. Chem. Phys.*, **1991**, 94 (2), 1360–1366. DOI: [10.1063/1.459993](https://doi.org/10.1063/1.459993).
- [72] Küchle, W.; Dolg, M.; Stoll, H.; Preuss, H. Energy-adjusted *ab initio* pseudopotentials for the rare earth elements. *Mol. Phys.*, **1991**, 74 (6), 1245–1263. DOI: [10.1063/1.456066](https://doi.org/10.1063/1.456066).
- [73] Dolg, M.; Fulde, P.; Küchle, W.; Neumann, C.-S.; Stoll, H. *J. Chem. Phys.*, **1991**, 94, 3011–3017.
- [74] Dolg, M.; Stoll, H.; Flad, H.-J.; Preuss, H. *J. Chem. Phys.*, **1992**, 97, 1162–1173.
- [75] Bergner, A.; Dolg, M.; Küchle, W.; Stoll, H.; Preuss, H. *Ab initio* energy-adjusted pseudopotentials for elements of groups 13–17. *Mol. Phys.*, **1993**, 80, 1431–1441. DOI: [10.1080/00268979300103121](https://doi.org/10.1080/00268979300103121).
- [76] Dolg, M.; Stoll, H.; Preuss, H.; Pitzer, R. M. *J. Phys. Chem.*, **1993**, 97, 5852–5859.
- [77] Dolg, M.; Stoll, H.; Preuss, H. *Theor. Chim. Acta*, **1993**, 85, 441–450.
- [78] Häußermann, U.; Dolg, M.; Stoll, H.; Preuss, H. *Mol. Phys.*, **1993**, 78, 1211–1224.
- [79] Küchle, W.; Dolg, M.; Stoll, H.; Preuss, H. Energy-adjusted pseudopotentials for the actinides: Parameter sets and test calculations for thorium and thorium monoxide. *J. Chem. Phys.*, **1994**, 100 (10), 7535–7542. DOI: [10.1063/1.466847](https://doi.org/10.1063/1.466847).
- [80] Nicklass, A.; Dolg, M.; Stoll, H.; Preuss, H. *J. Chem. Phys.*, **1995**, 102, 8942–8952.
- [81] Leininger, T.; Nicklass, A.; Stoll, H.; Dolg, M.; Schwerdtfeger, P. The accuracy of the pseudopotential approximation. II. A comparison of various core sizes for indium pseudopotentials in calculations for spectroscopic constants of InH, InF, and InCl. *J. Chem. Phys.*, **1996**, 105 (3), 1052–1059. DOI: [10.1063/1.471950](https://doi.org/10.1063/1.471950).
- [82] Leininger, T.; Nicklass, A.; Küchle, W.; Stoll, H.; Dolg, M.; Bergner, A. The accuracy of the pseudopotential approximation: Non-frozen-core effects for spectroscopic constants of alkali fluorides XF (X=K, Rb, Ca). *Chem. Phys. Lett.*, **1996**, 255 (4-6), 274–280. DOI: [10.1016/0009-2614\(96\)00382-X](https://doi.org/10.1016/0009-2614(96)00382-X).
- [83] Leininger, T.; Berning, A.; Nicklass, A.; Stoll, H.; Werner, H.-J.; Flad, H.-J. Spin-orbit interaction in heavy group 13 atoms and TlAr. *Chem. Phys.*, **1997**, 217 (1), 19–34. DOI: [10.1016/S0301-0104\(97\)00043-8](https://doi.org/10.1016/S0301-0104(97)00043-8).
- [84] Schautz, F.; Flad, H.-J.; Dolg, M. *Theor. Chem. Acc.*, **1998**, 99, 231.
- [85] Wang, Y.; Dolg, M. *Theor. Chem. Acc.*, **1998**, 100, 124.
- [86] Metz, Bernhard; Stoll, Hermann; Dolg, Michael. Small-Core Multiconfiguration-Dirac–Hartree–Fock-Adjusted Pseudopotentials for Post-d Main Group Elements: Application to PbH and PbO. *J. Chem. Phys.*, **2000**, 113, 2563–2569. DOI: [10.1063/1.1305880](https://doi.org/10.1063/1.1305880).

- [87] Metz, Bernhard; Schweizer, Markus; Stoll, Hermann; Dolg, Michael; Liu, Wenjian. Relativistic Energy-Consistent Pseudopotentials: Adjustments to Multi-Configuration Dirac–Hartree–Fock Data. *Theor. Chem. Acc.*, **2000**, 104, 22–28. DOI: [10.1007/s002140000187](https://doi.org/10.1007/s002140000187).
- [88] Martin, Jan M. L.; Sundermann, Andreas. Correlation Consistent Valence Basis Sets for Use with the Stuttgart–Dresden–Bonn Relativistic Effective Core Potentials: The Atoms Ga–Kr and In–Xe. *J. Chem. Phys.*, **2001**, 114 (8), 3408–3420. DOI: [10.1063/1.1337864](https://doi.org/10.1063/1.1337864).
- [89] Cao, X.; Dolg, M. Valence basis sets for relativistic energy-consistent small-core lanthanide pseudopotentials. *J. Chem. Phys.*, **2001**, 115, 7348. DOI: [10.1063/1.1406535](https://doi.org/10.1063/1.1406535).
- [90] Stoll, H.; Metz, B.; Dolg, M. *J. Comput. Chem.*, **2002**, 23, 767.
- [91] Cao, X.; Dolg, M. Segmented contraction scheme for small-core lanthanide pseudopotential basis sets. *J. Mol. Struct.: THEOCHEM*, **2002**, 581, 139. DOI: [10.1016/S0166-1280\(01\)00751-5](https://doi.org/10.1016/S0166-1280(01)00751-5).
- [92] Peterson, K. A. *J. Chem. Phys.*, **2003**, 119, 11099.
- [93] Peterson, K. A.; Figgen, D.; Goll, E.; Stoll, H.; Dolg, M. *J. Chem. Phys.*, **2003**, 119, 11113.
- [94] Figgen, D.; Rauhut, G.; Dolg, M.; Stoll, H. *Chem. Phys.*, **2005**, 311, 227.
- [95] Lim, I. S.; Schwerdtfeger, P.; Metz, B.; Stoll, H. All-electron and relativistic pseudopotential studies for the group 1 element polarizabilities from K to element 119. *J. Chem. Phys.*, **2005**, 122 (10), 104103. DOI: [10.1063/1.1856451](https://doi.org/10.1063/1.1856451).
- [96] Peterson, K. A.; Puzzarini, C. *Theor. Chem. Acc.*, **2005**, 114, 283.
- [97] Yang, J.; Dolg, M. *Theor. Chem. Acc.*, **2005**, 113, 212.
- [98] Lim, I. S.; Stoll, H.; Schwerdtfeger, P. Relativistic small-core energy-consistent pseudopotentials for the alkaline-earth elements from Ca to Ra. *J. Chem. Phys.*, **2006**, 124 (3), 034107. DOI: [10.1063/1.2148945](https://doi.org/10.1063/1.2148945).
- [99] Peterson, K. A.; Shepler, B. C.; Figgen, D.; Stoll, H. *J. Phys. Chem. A*, **2006**, 110, 13877.
- [100] Peterson, K. A.; Figgen, D.; Dolg, M.; Stoll, H. *J. Chem. Phys.*, **2007**, 126, 124101.
- [101] Moritz, Anna; Cao, Xiaoyan; Dolg, Michael. Quasirelativistic Energy-Consistent 5f-in-Core Pseudopotentials for Trivalent Actinide Elements. *Theor. Chem. Acc.*, **2007**, 117, 473–481. DOI: [10.1007/s00214-006-0180-7](https://doi.org/10.1007/s00214-006-0180-7).
- [102] Moritz, Anna; Dolg, Michael. Quasirelativistic Energy-Consistent 4f-in-Core Pseudopotentials for Trivalent Lanthanide Elements. *Theor. Chem. Acc.*, **2008**, 121, 297–304. DOI: [10.1007/s00214-008-0439-2](https://doi.org/10.1007/s00214-008-0439-2).
- [103] Hülse, M.; Weigand, A.; Dolg, M. *Theor. Chem. Acc.*, **2009**, 122, 23.
- [104] Figgen, D.; Peterson, K. A.; Dolg, M.; Stoll, H. *J. Chem. Phys.*, **2009**, 130, 164108.
- [105] Weigand, A.; Cao, X.; Yang, J.; Dolg, M. *Theor. Chem. Acc.*, **2010**, 126, 117–127.
- [106] Flores-Moreno, R.; Alvares-Mendez, R. J.; Vela, A.; Köster, A. M. *J. Comput. Chem.*, **2006**, 27, 1009.
- [107] Giordano, L.; Pacchioni, G.; Bredow, T.; Sanz, J. F. *Surf. Sci.*, **2001**, 471, 21.
- [108] Facility, Molecular Science Computing. Extensible Computational Chemistry Environment Basis Set Database. **2000**. URL: <http://www.emsl.pnl.gov:2080/forms/basisform.html>.
- [109] Mitin, Alexander V.; Hirsch, Gernot; Buenker, Robert J. A Mean-Field Spin–Orbit Method Applicable to Correlated Wavefunctions. *Chem. Phys. Lett.*, **1996**, 259, 151–158. DOI: [10.1016/0009-2614\(96\)00119-4](https://doi.org/10.1016/0009-2614(96)00119-4).
- [110] Mitin, Alexander V.; Hirsch, Gernot; Buenker, Robert J. A Mean-Field Spin–Orbit Method Applicable to Correlated Wavefunctions. *J. Comput. Chem.*, **1997**, 18, 1200–1210. DOI: [10.1002/\(SICI\)1096-987X\(19970715\)18:9<1200::AID-JCC8>3.0.CO;2-2](https://doi.org/10.1002/(SICI)1096-987X(19970715)18:9<1200::AID-JCC8>3.0.CO;2-2).
- [111] Whitten, J. L. *J. Chem. Phys.*, **1973**, 58, 4496. DOI: [10.1063/1.1679012](https://doi.org/10.1063/1.1679012).
- [112] Baerends, E. J.; Ellis, D. E.; Ros, P. Self-consistent molecular Hartree–Fock–Slater calculations I. The computational procedure. *Chem. Phys.*, **1973**, 2, 41. DOI: [10.1016/0301-0104\(73\)80059-X](https://doi.org/10.1016/0301-0104(73)80059-X).
- [113] Dunlap, B. I.; Connolly, J. W. D.; Sabin, J. R. *J. Chem. Phys.*, **1979**, 71, 3396.
- [114] Van Alsenoy, C. *J. Comput. Chem.*, **1988**, 9, 620.

- [115] Kendall, Rick A.; Früchtel, Herbert A. The Impact of the Resolution of the Identity Approximate Integral Method on Modern Ab Initio Algorithm Development. *Theor. Chem. Acc.*, **1997**, 97, 158–163. DOI: 10.1007/s002140050249.
- [116] Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.*, **1995**, 240, 283.
- [117] Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.*, **1997**, 97, 119.
- [118] Vahtras, O.; Almlöf, J.; Feyereisen, M. W. *Chem. Phys. Lett.*, **1993**, 213, 514.
- [119] Neese, F.; Wennmohs, F.; Hansen, A.; Becker, U. *Chem. Phys.*, **2009**, 356, 98–109.
- [120] Helmich-Paris, Benjamin; de Souza, Bernardo; Neese, Frank; Izsák, Róbert. An improved chain of spheres for exchange algorithm. *J. Chem. Phys.*, **2021**, 155 (10), 104109. DOI: 10.1063/5.0058766.
- [121] Helmich-Paris, Benjamin. A trust-region augmented Hessian implementation for state-specific and state-averaged CASSCF wave functions. *J. Chem. Phys.*, **2022**, 156 (20), 204104. arXiv:10.1063/5.0090447, DOI: 10.1063/5.0090447.
- [122] Kossmann, Simone; Neese, Frank. Comparison of two efficient approximate Hartree–Fock approaches. *Chem. Phys. Lett.*, **2009**, 481 (4–6), 240–243. DOI: 10.1016/j.cplett.2009.10.007.
- [123] Treutler, O.; Ahlrichs, R. *J. Chem. Phys.*, **1994**, 102, 346.
- [124] Kruse, Holger; Grimme, Stefan. A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree–Fock and density functional theory calculations for large systems. *J. Chem. Phys.*, **2012**, 136 (15), 154101. DOI: 10.1063/1.3700154.
- [125] Kruse, Holger; Goerigk, Lars; Grimme, Stefan. Why the Standard B3LYP/6-31G* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problem. *J. Org. Chem.*, **2012**, 77 (23), 10824–10834. DOI: 10.1021/jo301927e.
- [126] van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.*, **1994**, 101, 9783–9792.
- [127] van Wüllen, C. *J. Chem. Phys.*, **1998**, 109, 392–399.
- [128] Sandhoefer, B.; Neese, F. One-electron contributions to the g-tensor for second-order Douglas–Kroll–Hess theory. *J. Chem. Phys.*, **2012**, 137, 094102.
- [129] Peng, Daoling; Middelndorf, Nils; Weigend, Florian; Reiher, Markus. An efficient implementation of two-component relativistic exact-decoupling methods for large molecules. *J. Chem. Phys.*, **2013**, 138 (18), 184105. DOI: 10.1063/1.4803693.
- [130] Franzke, Yannick J.; Middelndorf, Nils; Weigend, Florian. Efficient implementation of one- and two-component analytical energy gradients in exact two-component theory. *J. Chem. Phys.*, **2018**, 148 (10), 104110. DOI: 10.1063/1.5022153.
- [131] Franzke, Yannick J.; Yu, Jason M. Hyperfine Coupling Constants in Local Exact Two-Component Theory. *J. Chem. Theory Comput.*, **2022**, 18 (1), 323–343. DOI: 10.1021/acs.jctc.1c01027.
- [132] Franzke, Yannick J.; Mack, Fabian; Weigend, Florian. NMR Indirect Spin–Spin Coupling Constants in a Modern Quasi-Relativistic Density Functional Framework. *J. Chem. Theory Comput.*, **2021**, 17 (7), 3974–3994. DOI: 10.1021/acs.jctc.1c00167.
- [133] Franzke, Yannick J.; Weigend, Florian. NMR Shielding Tensors and Chemical Shifts in Scalar-Relativistic Local Exact Two-Component Theory. *J. Chem. Theory Comput.*, **2019**, 15 (2), 1028–1043. DOI: 10.1021/acs.jctc.8b01084.
- [134] Cheng, Lan; Gauss, Jürgen. Analytic energy gradients for the spin-free exact two-component theory using an exact block diagonalization for the one-electron Dirac Hamiltonian. *J. Chem. Phys.*, **2011**, 135 (8), 084114. DOI: 10.1063/1.3624397.
- [135] Cheng, Lan; Gauss, Jürgen. Analytic second derivatives for the spin-free exact two-component theory. *J. Chem. Phys.*, **2011**, 135 (24), 244104. DOI: 10.1063/1.3667202.
- [136] Cheng, Lan; Gauss, Jürgen; Stanton, John F. Treatment of scalar-relativistic effects on nuclear magnetic shieldings using a spin-free exact-two-component approach. *J. Chem. Phys.*, **2013**, 139 (5), 054105. DOI: 10.1063/1.4816130.

- [137] Peng, Daoling; Reiher, Markus. Local relativistic exact decoupling. *J. Chem. Phys.*, **2012**, 136 (24), 244108. DOI: [10.1063/1.4729788](https://doi.org/10.1063/1.4729788).
- [138] Visscher, L.; Dyall, K. G. *Atom. Data Nucl. Data Tabl.*, **1997**, 67, 207.
- [139] Barone, V.; Cossi, M. Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model. *J. Phys. Chem. A*, **1998**, 102, 1995–2001. DOI: [10.1021/jp9716997](https://doi.org/10.1021/jp9716997).
- [140] Garcia-Ratés, M.; Neese, F. Effect of the Solute Cavity on the Solvation Energy and its Derivatives within the Framework of the Gaussian Charge Scheme. *J. Comput. Chem.*, **2020**, 41 (9), 922–939. DOI: [10.1002/jcc.26139](https://doi.org/10.1002/jcc.26139).
- [141] Marenich, Aleksandr V.; Cramer, Christopher J.; Truhlar, Donald G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B*, **2009**, 113 (18), 6378–6396. DOI: [10.1021/jp810292n](https://doi.org/10.1021/jp810292n).
- [142] Gerlach, Thomas; Müller, Simon; González de Castilla, Andrés; Smirnova, Irina. An Open Source COSMO-RS Implementation and Parameterization Supporting the Efficient Implementation of Multiple Segment Descriptors. *Fluid Phase Equil.*, **2022**, 560, 113472.
- [143] York, D. M.; Karplus, M. *J. Phys. Chem. A*, **1999**, 103, 11060–11079.
- [144] Pascual-Ahuir, J. L.; Silla, E. *J. Comput. Chem.*, **1990**, 11, 1047–1060.
- [145] Pascual-Ahuir, J. L.; Silla, E.; Tunon, I. *J. Comput. Chem.*, **1991**, 12, 1077–1088.
- [146] Pascual-Ahuir, J. L.; Silla, E.; Tunon, I. *J. Comput. Chem.*, **1994**, 15, 1127–1138.
- [147] Lange, Adrian W.; Herbert, John M. A smooth, nonsingular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approach. *J. Chem. Phys.*, **2010**, 133 (24), 244111. DOI: [10.1063/1.3511297](https://doi.org/10.1063/1.3511297).
- [148] Haynes, W. M.; Lide, D. R.; Bruno, T. J. *Handbook of Chemistry and Physics*. CRC Press, 95th edition, **2014**. ISBN 978-1-4822-0868-9.
- [149] Stahn, M.; Ehlert, S.; Grimme, S. Extended Conductor-like Polarizable Continuum Solvation Model (CPCM-X) for Semiempirical Methods. *J. Phys. Chem. A*, **2023**, 127, 7036–7043. DOI: [10.1021/acs.jpca.3c04382](https://doi.org/10.1021/acs.jpca.3c04382).
- [150] Bondi, A. *J. Phys. Chem.*, **1964**, 68, 441–451.
- [151] Mantina, M.; Chamberlin, A. C.; Valero, R.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. A*, **2009**, 113, 5806–5812.
- [152] Klamt, A.; Eckert, F. COSMO-RS: a novel and efficient method for the a priori prediction of thermophysical data of liquids. *Fluid Phase Equil.*, **2000**, 172, 43–72. DOI: [10.1016/S0378-3812\(00\)00357-5](https://doi.org/10.1016/S0378-3812(00)00357-5).
- [153] Truong, T. N.; Stefanovich, E. V. *Chem. Phys. Lett.*, **1995**, 240, 253–260.
- [154] Pierotti, R. A. *Chem. Rev.*, **1976**, 76, 717.
- [155] Claverie, P.; Daudey, J. P.; Langlet, J.; Pullman, B.; Plazzola, D.; Huron, M. J. Studies of solvent effects. 1. Discrete, continuum, and discrete–continuum models and their comparison for some simple cases: ammonium(1+) ion, methanol, and substituted ammonium(1+) ion. *J. Phys. Chem.*, **1978**, 82, 405–418. DOI: [10.1021/j100493a008](https://doi.org/10.1021/j100493a008).
- [156] Pye, C. C.; Ziegler, T. *Theor. Chem. Acc.*, **1999**, 101, 396.
- [157] Engelage, Elric.; Schulz, Nils; Flemming, Heinen; Huber, Stefan M.; Truhlar, Donald G.; Cramer, Christopher J. Refined SMD Parameters for Bromine and Iodine Accurately Model Halogen-Bonding Interactions in Solution. *Chem. Eur. J.*, **2018**, 24, 15983.
- [158] Plett, Christoph; Stahn, Marcel; Bursch, Markus; Mewes, Jan-Michael; Grimme, Stefan. Improving Quantum Chemical Solvation Models by Dynamic Radii Adjustment for Continuum Solvation Method (DRACO). *J. Phys. Chem. Lett.*, **2024**, 15, 2462.
- [159] Caldeweyher, Eike; Ehlert, Sebastian; Hansen, Andreas; Neugebauer, Hagen; Spicher, Sebastian; Bannwarth, Christoph; Grimme, Stefan. A Generally Applicable Atomic-Charge Dependent London Dispersion Correction. *J. Chem. Phys.*, **2019**, 150 (15), 154122. arXiv:[10.1063/1.5090222](https://arxiv.org/abs/10.1063/1.5090222), DOI: [10.1063/1.5090222](https://doi.org/10.1063/1.5090222).

- [160] Müller, Marcel; Hansen, Andreas; Grimme, Stefan. An atom-in-molecule adaptive polarized valence single- ζ atomic orbital basis for electronic structure calculations. *J. Chem. Phys.*, **2023**, 159, 164108.
- [161] Bannwarth, Christoph; Ehlert, Sebastian; Grimme, Stefan. GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. *J. Chem. Theory Comput.*, **2019**, 15 (3), 1652–1671. DOI: [10.1021/acs.jctc.8b01176](https://doi.org/10.1021/acs.jctc.8b01176).
- [162] 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](https://doi.org/10.1002/jcc.70099).
- [163] Müller, Simon; Nevolianis, Thomas; Garcia-Ratés, Miquel; Riplinger, Christoph; Leonhard, Kai; Smirnova, Irina. Predicting solvation free energies for neutral molecules in any solvent with openCOSMO-RS. *Fluid Phase Equilibria*, **2025**, 589, 114250. DOI: [10.1016/j.fluid.2024.114250](https://doi.org/10.1016/j.fluid.2024.114250).
- [164] Klamt, Andreas. Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena. *J. Phys. Chem.*, **1995**, 99, 2224–2235.
- [165] Klamt, Andreas; Volker, Jonas; Bürger, Thorsten; Lohrenz, John C. W. Refinement and Parametrization of COSMO-RS. *J. Phys. Chem. A*, **1998**, 102, 5074–5085.
- [166] Cammi, R. Quantum cluster theory for the polarizable continuum model. I. The CCSD level with analytical first and second derivatives. *J. Chem. Phys.*, **2009**, 131, 164104. DOI: [10.1063/1.3245400](https://doi.org/10.1063/1.3245400).
- [167] Caricato, M. CCSD-PCM: Improving upon the reference reaction field approximation at no cost. *J. Chem. Phys.*, **2011**, 135, 074113. DOI: [10.1063/1.3624373](https://doi.org/10.1063/1.3624373).
- [168] Garcia-Ratés, M.; Becker, U.; Neese, F. Implicit Solvation in Domain Based Pair Natural Orbital Coupled Cluster (DLPNO-CCSD) Theory. *J. Comput. Chem.*, **2021**, 42 (27), 1959–1973. DOI: [10.1002/jcc.26726](https://doi.org/10.1002/jcc.26726).
- [169] Almlöf, J. Faegri, K.; Korsell, K. Principles for a direct SCF approach to LCAO-MO ab-initio calculations. *J. Comput. Chem.*, **1982**, 3, 385. DOI: [10.1002/jcc.540030314](https://doi.org/10.1002/jcc.540030314).
- [170] Almlöf, J.; Taylor, P. R. Computational Aspects of Direct SCF and MCSCF Methods. In Dykstra, C. E., editor, *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules*, pages 107. Springer, **1984**. DOI: [10.1007/978-94-009-6451-5](https://doi.org/10.1007/978-94-009-6451-5).
- [171] Almlöf, J. Direct Methods in Electronic Structure Theory. In Yarkony, D. R., editor, *Modern Electronic Structure Theory*, pages 110. World Scientific, **1995**. DOI: [10.1142/1957](https://doi.org/10.1142/1957).
- [172] Häser, M.; Ahlrichs, R. *J. Comput. Chem.*, **1989**, 10, 104.
- [173] Seeger, R.; Pople, J. A. *J. Chem. Phys.*, **1977**, 66, 3045.
- [174] Bauernschmitt, R.; Ahlrichs, R. Stability analysis for solutions of the closed shell Kohn-Sham equation. *J. Chem. Phys.*, **1996**, 104, 9047. DOI: [10.1063/1.471637](https://doi.org/10.1063/1.471637).
- [175] Shaik, Sason; Ramanan, Rajeev; Danovich, David; Mandal, Debasish. Structure and reactivity/selectivity control by oriented-external electric fields. *Chem. Soc. Rev.*, **2018**, 47, 5125–5145. DOI: [10.1039/C8CS00354H](https://doi.org/10.1039/C8CS00354H).
- [176] Mulliken, R. S. Report on Notation for the Spectra of Polyatomic Molecules. *J. Chem. Phys.*, **1955**, 23 (11), 1997–2011. DOI: [10.1063/1.1740655](https://doi.org/10.1063/1.1740655).
- [177] Schutte, C. J. H.; Bertie, J. E.; Bunker, P. R.; Hougen, J. T.; Mills, I. M.; Watson, J. K. G.; Winnewisser, B. P. Notations and conventions in molecular spectroscopy: Part 2. Symmetry notation (IUPAC Recommendations 1997). *Pure & Appl. Chem.*, **1997**, 69 (8), 1641–1649. DOI: [10.1351/pac199769081641](https://doi.org/10.1351/pac199769081641).
- [178] Amos, A. T.; Hall, G. G. Single determinant wave functions. *Proc. R. Soc. Ser. A.*, **1961**, 263, 483. DOI: [10.1098/rspa.1961.0175](https://doi.org/10.1098/rspa.1961.0175).
- [179] King, Harry F.; Stanton, Richard E.; Kim, Hojing; Wyatt, Robert E.; Parr, Robert G. Corresponding Orbitals and the Nonorthogonality Problem in Molecular Quantum Mechanics. *J. Chem. Phys.*, **1967**, 47, 1936–1941. DOI: [10.1063/1.1712221](https://doi.org/10.1063/1.1712221).
- [180] Szabo, A.; Ostlund, N. S. *Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory*. Dover Publications, **1989**. ISBN 978-0-486-69186-2.
- [181] Dewar, M. J. S.; Hashmall, J. A.; Venier, C. G. *J. Am. Chem. Soc.*, **1968**, 90, 1953.

- [182] McWeeny, R. SCF Theory for Excited States. I. *Mol. Phys.*, **1974**, 28 (5), 1273–1282. DOI: [10.1080/00268977400102581](https://doi.org/10.1080/00268977400102581).
- [183] Brobowicz, F. W.; Goddard, W. A. In III, H. F. Schaefer, editor, *Methods of Electronic Structure Theory*, pages 79. Plenum Press, **1977**.
- [184] Carbo, R.; Riera, J. M. *A General SCF Theory. Lecture Notes in Chemistry*. Springer Verlag, **1978**.
- [185] Binkley, J. S.; Pople, J. A.; Dobosh, P. A. The calculation of spin-restricted single-determinant wavefunctions. *Mol. Phys.*, **1974**, 28, 1423. DOI: [10.1080/00268977400102701](https://doi.org/10.1080/00268977400102701).
- [186] Edwards, W. D.; Zerner, M. C. *Theor. Chim. Acta*, **1987**, 72, 347.
- [187] Muller, R. P.; Langlois, J. M.; Ringnalda, M. N.; Friesner, R. A.; Goddard, W. A. A Generalized Direct Inversion in the Iterative Subspace Approach for Generalized Valence Bond Wavefunctions. *J. Chem. Phys.*, **1994**, 100, 1226–1239. DOI: [10.1063/1.466639](https://doi.org/10.1063/1.466639).
- [188] Bofill, J. M.; Bono, H.; Rubio, J. Analysis of the convergence of the general coupling operator method for one-configuration-type wave functions. *J. Comput. Chem.*, **1998**, 19, 368. DOI: [10.1002/\(SICI\)1096-987X\(199802\)19:3<368::AID-JCC10>3.0.CO;2-E](https://doi.org/10.1002/(SICI)1096-987X(199802)19:3<368::AID-JCC10>3.0.CO;2-E).
- [189] Stavrev, K. K.; Zerner, M. C. Spin-averaged Hartree–Fock procedure for spectroscopic calculations: The absorption spectrum of Mn²⁺ in ZnS crystals. *Int. J. Quant. Chem.*, **1997**, 65 (5), 877–884. DOI: [10.1002/\(SICI\)1097-461X\(1997\)65:5<877::AID-QUA51>3.0.CO;2-T](https://doi.org/10.1002/(SICI)1097-461X(1997)65:5<877::AID-QUA51>3.0.CO;2-T).
- [190] Zerner, M. C. *Int. J. Quant. Chem.*, **1989**, 35, 567.
- [191] Leyser da Costa Gouveia, Tiago; Maganas, Dimitrios; Neese, Frank. Restricted Open-Shell Hartree–Fock Method for a General Configuration State Function Featuring Arbitrarily Complex Spin-Couplings. *J. Phys. Chem. A*, **2024**, 128 (25), 5041–5053. PMID: 38886177. DOI: [10.1021/acs.jpca.4c00688](https://doi.org/10.1021/acs.jpca.4c00688).
- [192] Hartree, D. R. The Wave Mechanics of an Atom with a Non-Coulomb Central Field. Part I. Theory and Methods. *Proc. Cambridge Phil. Soc.*, **1928**, 24, 89–110. DOI: [10.1017/S0305004100011919](https://doi.org/10.1017/S0305004100011919).
- [193] Slater, J. C. The Theory of Complex Spectra. *Phys. Rev.*, **1929**, 34, 1293–1322. DOI: [10.1103/PhysRev.34.1293](https://doi.org/10.1103/PhysRev.34.1293).
- [194] Fock, V. Näherungsmethode zur Lösung des quantenmechanischen Mehrkörperproblems. *Z. Phys.*, **1930**, 61, 126–148. DOI: [10.1007/BF01340294](https://doi.org/10.1007/BF01340294).
- [195] Perdew, John P.; Schmidt, Karla. Jacob’s ladder of density functional approximations for the exchange-correlation energy. *AIP Conf. Proc.*, **2001**, 577 (1), 1–20. DOI: [10.1063/1.1390175](https://doi.org/10.1063/1.1390175).
- [196] Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.*, **1980**, 58, 1200.
- [197] Perdew, J. P.; Wang, Y. *Phys. Rev. B*, **1992**, 45, 13244.
- [198] Becke, A. D. Density-functional exchange-energy approximation with correct asymptotic behavior. *Phys. Rev. A*, **1988**, 38, 3098. DOI: [10.1103/PhysRevA.38.3098](https://doi.org/10.1103/PhysRevA.38.3098).
- [199] Perdew, J. P. *Phys. Rev. B*, **1986**, 33, 8822.
- [200] Miehlich, Burkhard; Savin, Andreas; Stoll, Hermann; Preuss, Heinzwerner. Results obtained with the correlation energy density functionals of Becke and Lee, Yang and Parr. *Chem. Phys. Lett*, **1989**, 157 (3), 200–206. DOI: [10.1016/0009-2614\(89\)87234-3](https://doi.org/10.1016/0009-2614(89)87234-3).
- [201] Handy, Nicholas C.; Cohen, Aron J. Left-right correlation energy. *Mol. Phys.*, **2001**, 99 (5), 403–412. DOI: [10.1080/00268970010018431](https://doi.org/10.1080/00268970010018431).
- [202] Gill, P. M. W. *Mol. Phys.*, **1996**, 89, 433. DOI: [10.1080/002689796173813](https://doi.org/10.1080/002689796173813).
- [203] Xu, Xin; Goddard, III, William A. *Proc. Nat. Acad. Sci.*, **2004**, 101, 2673.
- [204] Germany), W. E. Heraeus Seminar (75th 1991 Gaussig. *Electronic structure of solids '91: proceedings of the 75. WE-Heraeus-Seminar and 21st Annual International Symposium on Electronic Structure of Solids held in Gaussig (Germany), March 11-15, 1991*. Akademie Verlag, Berlin, 1st ed. edition, **1991**. ISBN 978-3-05-501504-5. Open Library ID: OL1778449M.

- [205] Adamo, C.; Barone, V. Exchange functionals with improved long-range behavior and adiabatic connection methods without adjustable parameters: The mPW and mPW1PW models. *J. Chem. Phys.*, **1998**, 108, 664. DOI: 10.1063/1.475428.
- [206] Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.*, **1996**, 77, 3865.
- [207] Hammer, B.; Hansen, L. B.; Nørskov, J. K. *Phys. Rev. B*, **1999**, 59, 7413.
- [208] Zhang, Y.; Yang, W. *Phys. Rev. Lett.*, **1998**, 80, 890.
- [209] Murray, Éamonn D.; Lee, Kyuho; Langreth, David C. Investigation of Exchange Energy Density Functional Accuracy for Interacting Molecules. *J. Chem. Theory Comput.*, **2009**, 5 (10), 2754–2762. DOI: 10.1021/ct900365q.
- [210] Brandenburg, Jan Gerit; Bannwarth, Christoph; Hansen, Andreas; Grimme, Stefan. B97-3c: A Revised Low-Cost Variant of the B97-D Density Functional Method. *J. Chem. Phys.*, **2018**, 148 (6), 064104. DOI: 10.1063/1.5012601.
- [211] Mardirossian, Narbe; Head-Gordon, Martin. Mapping the genome of meta-generalized gradient approximation density functionals: The search for B97M-V. *J. Chem. Phys.*, **2015**, 142, 074111. DOI: 10.1063/1.4907719.
- [212] Najibi, A.; Goerigk, L. *J. Chem. Theory Comput.*, **2018**, 14, 5725.
- [213] Najibi, A.; Goerigk, L. DFT-D4 Counterparts of Leading Meta-Generalized-Gradient Approximation and Hybrid Density Functionals for Energetics and Geometries. *J. Comput. Chem.*, **2020**, 41, 2562–2572. DOI: 10.1002/jcc.26411.
- [214] Sun, Jianwei; Ruzsinszky, Adrienn; Perdew, John P. Strongly Constrained and Appropriately Normed Semilocal Density Functional. *Phys. Rev. Lett.*, **2015**, 115 (3), 036402. DOI: 10.1103/PhysRevLett.115.036402.
- [215] Bartók, Albert P.; Yates, Jonathan R. Regularized SCAN Functional. *J. Chem. Phys.*, **2019**, 150 (16), 161101. DOI: 10.1063/1.5094646.
- [216] Furness, James W.; Kaplan, Aaron D.; Ning, Jinliang; Perdew, John P.; Sun, Jianwei. Accurate and Numerically Efficient r²SCAN Meta-Generalized Gradient Approximation. *J. Phys. Chem. Lett.*, **2020**, 11 (19), 8208–8215. DOI: 10.1021/acs.jpclett.0c02405.
- [217] Zhao, Yan; Truhlar, Donald G. A new local density functional for main-group thermochemistry, transition metal bonding, thermochemical kinetics, and noncovalent interactions. *J. Chem. Phys.*, **2006**, 125 (19), 194101. DOI: 10.1063/1.2370993.
- [218] Staroverov, V. N.; Scuseria, G. E.; Tao, J.; Perdew, J. P. *J. Chem. Phys.*, **2003**, 119, 12129.
- [219] Perdew, John P.; Ruzsinszky, Adrienn; Csonka, Gábor I.; Constantin, Lucian A.; Sun, Jianwei. Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry. *Phys. Rev. Lett.*, **2009**, 103, 026403. DOI: 10.1103/PhysRevLett.103.026403.
- [220] Perdew, John P.; Ruzsinszky, Adrienn; Csonka, Gábor I.; Constantin, Lucian A.; Sun, Jianwei. Erratum: Workhorse Semilocal Density Functional for Condensed Matter Physics and Quantum Chemistry [Phys. Rev. Lett. 103, 026403 (2009)]. *Phys. Rev. Lett.*, **2011**, 106, 179902. DOI: 10.1103/PhysRevLett.106.179902.
- [221] Grimme, Stefan; Hansen, Andreas; Ehlert, Sebastian; Mewes, Jan-Michael. r2SCAN-3c: A “Swiss Army Knife” Composite Electronic-Structure Method. *J. Chem. Phys.*, **2021**, 154 (6), 064103. arXiv:10.1063/5.0040021, DOI: 10.1063/5.0040021.
- [222] Ahlrichs, R.; Bär, M.; Baron, H. P.; Bauernschmitt, R.; Böcker, S.; Ehrig, M.; Eichkorn, K.; Elliott, S.; Furche, F.; Haase, F.; Häser, M.; Horn, H.; Huber, C.; Huniar, U.; Kattaneck, M.; Kölmel, C.; Kollwitz, M.; May, K.; Ochsenfeld, C.; Öhm, H.; Schäfer, A.; Schneider, U.; Treutler, O.; von Arnim, M.; Weigend, F.; Weis, P.; Weiss, H. *TurboMole - Program System for Ab Initio Electronic Structure Calculations, Version 5.2*. Universität Karlsruhe, Karlsruhe, Germany, **2000**.
- [223] Ahlrichs, R. In Schleyer, P. v. R., editor, *Encyclopedia of Computational Chemistry*, pages 3123. John Wiley and Sons, **1998**. DOI: 10.1002/0470845015.
- [224] Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. Electronic structure calculations on workstation computers: The program system turbomole. *Chem. Phys. Lett.*, **1989**, 162, 165. DOI: 10.1016/0009-2614(89)85118-8.

- [225] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Baboul, A. G.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Andres, J. L.; Gonzalez, C.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98, Revision A.8*. Gaussian, Inc., Pittsburgh PA, **1998**.
- [226] Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B*, **1988**, 37 (2), 785–789. DOI: [10.1103/PhysRevB.37.785](https://doi.org/10.1103/PhysRevB.37.785).
- [227] Becke, A. D. A new mixing of Hartree-Fock and local density-functional theories. *J. Chem. Phys.*, **1993**, 98, 1372. DOI: [10.1063/1.464304](https://doi.org/10.1063/1.464304).
- [228] Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.*, **1993**, 98, 5648. DOI: [10.1063/1.464913](https://doi.org/10.1063/1.464913).
- [229] Adamo, C.; Barone, V. Toward Reliable Density Functional Methods without Adjustable Parameters: The PBE0 Model. *J. Chem. Phys.*, **1999**, 110, 6158. DOI: [10.1063/1.478522](https://doi.org/10.1063/1.478522).
- [230] Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab Initio Calculation of Vibrational Absorption and Circular Dichroism Spectra Using Density Functional Force Fields. *J. Phys. Chem.*, **1994**, 98, 11623. DOI: [10.1021/j100096a001](https://doi.org/10.1021/j100096a001).
- [231] Ernzerhof, M. In Joubert, D. P., editor, *Density Functionals: Theory and Applications*. Springer Verlag, **1998**.
- [232] Adamo, C.; Barone, V. Toward reliable adiabatic connection models free from adjustable parameters. *Chem. Phys. Lett.*, **1997**, 274 (1), 242–250. DOI: [10.1016/S0009-2614\(97\)00651-9](https://doi.org/10.1016/S0009-2614(97)00651-9).
- [233] aron J. Cohen; Handy, Nicholas C. Dynamic correlation. *Mol. Phys.*, **2001**, 99 (7), 607–615. DOI: [10.1080/00268970010023435](https://doi.org/10.1080/00268970010023435).
- [234] Goerigk, Lars; Grimme, Stefan. A thorough benchmark of density functional methods for general main group thermochemistry, kinetics, and noncovalent interactions. *Phys. Chem. Chem. Phys.*, **2011**, 13, 6670–6688. DOI: [10.1039/C0CP02984J](https://doi.org/10.1039/C0CP02984J).
- [235] Zhao, Yan; Truhlar, Donald G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.*, **2008**, 120 (1-3), 215–241. DOI: [10.1007/s00214-007-0310-x](https://doi.org/10.1007/s00214-007-0310-x).
- [236] Zhao, Y.; Truhlar, D. G. *J. Phys. Chem. A*, **2005**, 109, 5656–5667.
- [237] Grimme, Stefan. Accurate Calculation of the Heats of Formation for Large Main Group Compounds with Spin-Component Scaled MP2 Methods. *J. Phys. Chem. A*, **2005**, 109 (13), 3067–3077. DOI: [10.1021/jp050036j](https://doi.org/10.1021/jp050036j).
- [238] Bursch, Markus; Neugebauer, Hagen; Ehlert, Sebastian; Grimme, Stefan. Dispersion corrected r²SCAN based global hybrid functionals: r²SCANh, r²SCAN0, and r²SCAN50. *J. Chem. Phys.*, **2022**, 156 (13), 134105. DOI: [10.1063/5.0086040](https://doi.org/10.1063/5.0086040).
- [239] Grimme, S.; Brandenburg, J. G.; Bannwarth, C.; Hansen, A. Consistent structures and interactions by density functional theory with small atomic orbital basis sets. *J. Chem. Phys.*, **2015**, 143, 054107. DOI: [10.1063/1.4927476](https://doi.org/10.1063/1.4927476).
- [240] Pracht, Philipp; Grant, David F.; Grimme, Stefan. Comprehensive Assessment of GFN Tight-Binding and Composite Density Functional Theory Methods for Calculating Gas-Phase Infrared Spectra. *J. Chem. Theory Comput.*, **2020**, 16 (11), 7044–7060. DOI: [10.1021/acs.jctc.0c00877](https://doi.org/10.1021/acs.jctc.0c00877).
- [241] Iikura, H.; Tsuneda, T.; Yanai, T.; Hirao, K. A long-range correction scheme for generalized-gradient-approximation exchange functionals. *J. Chem. Phys.*, **2001**, 115, 3540–3544. DOI: [10.1063/1.1383587](https://doi.org/10.1063/1.1383587).
- [242] Yanai, T.; Tew, D. P.; Handy, N. C. *Chem. Phys. Lett.*, **2004**, 393, 51–57.
- [243] Chai, J.-D.; Head-Gordon, M. *J. Chem. Phys.*, **2008**, 128, 084106.

- [244] Mardirossian, Narbe; Head-Gordon, Martin. ω B97X-V: A 10-parameter, range-separated hybrid, generalized gradient approximation density functional with nonlocal correlation, designed by a survival-of-the-fittest strategy. *Phys. Chem. Chem. Phys.*, **2014**, 16 (21), 9904–9924. DOI: [10.1039/C3CP54374A](https://doi.org/10.1039/C3CP54374A).
- [245] Lin, Y.-S.; Li, G.-D.; Mao, S.-P.; Chai, J.-D. Long-Range Corrected Hybrid Density Functionals with Improved Dispersion Corrections. *J. Chem. Theory Comput.*, **2013**, 9, 263–272. DOI: [10.1021/ct300715s](https://doi.org/10.1021/ct300715s).
- [246] Tawada, Y.; Tsuneda, T.; Yanagisawa, S.; Yanai, T.; Hirao, K. *J. Chem. Phys.*, **2004**, 120, 8425–8433.
- [247] Mardirossian, Narbe; Head-Gordon, Martin. ω B97M-V: A combinatorially optimized, range-separated hybrid, meta-GGA density functional with VV10 nonlocal correlation. *J. Chem. Phys.*, **2016**, 144, 214110. DOI: [10.1063/1.4952647](https://doi.org/10.1063/1.4952647).
- [248] Wittmann, Lukas; Neugebauer, Hagen; Grimme, Stefan; Bursch, Markus. Dispersion-corrected r^2 SCAN based double-hybrid functionals. *J. Chem. Phys.*, **2023**, 159 (22), 224103. DOI: [10.1063/5.0174988](https://doi.org/10.1063/5.0174988).
- [249] Grimme, S. *J. Chem. Phys.*, **2006**, 124, 034108.
- [250] Goerigk, L.; Grimme, S. *J. Chem. Theory Comput.*, **2011**, 7, 291–309.
- [251] Kozuch, Sebastian; Gruzman, David; Martin, Jan M. L. DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction. *J. Phys. Chem. C*, **2010**, 114 (48), 20801–20808. DOI: [10.1021/jp1070852](https://doi.org/10.1021/jp1070852).
- [252] Kozuch, Sebastian; Martin, Jan M. L. DSD-PBEP86: In Search of the Best Double-Hybrid DFT with Spin-Component Scaled MP2 and Dispersion Corrections. *Phys. Chem. Chem. Phys.*, **2011**, 13 (45), 20104–20107. DOI: [10.1039/C1CP22592H](https://doi.org/10.1039/C1CP22592H).
- [253] Kozuch, Sebastian; Martin, Jan M. L. Spin-component-scaled Double Hybrids: An Extensive Search for the Best Fifth-rung Functionals Blending DFT and Perturbation Theory. *J. Comput. Chem.*, **2013**, 34 (27), 2327–2344. DOI: [10.1002/jcc.23391](https://doi.org/10.1002/jcc.23391).
- [254] Santra, Golokesh; Cho, Minsik; Martin, Jan M. L. Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with xDSD as a Special Case. *J. Phys. Chem. A*, **2021**, 125 (21), 4614–4627. DOI: [10.1021/acs.jpca.1c01294](https://doi.org/10.1021/acs.jpca.1c01294).
- [255] Zhang, Ying; Xu, Xin; Goddard, William A. Doubly hybrid density functional for accurate descriptions of nonbond interactions, thermochemistry, and thermochemical kinetics. *Proc. Natl. Acad. Sci. USA*, **2009**, 106 (13), 4963–4968. DOI: [10.1073/pnas.0901093106](https://doi.org/10.1073/pnas.0901093106).
- [256] Mardirossian, Narbe; Head-Gordon, Martin. Survival of the most transferable at the top of Jacob's ladder: Defining and testing the ω B97M(2) double hybrid density functional. *J. Chem. Phys.*, **2018**, 148 (24), 241736. DOI: [10.1063/1.5025226](https://doi.org/10.1063/1.5025226).
- [257] Neugebauer, Hagen; Pinski, Peter; Grimme, Stefan; Neese, Frank; Bursch, Markus. Assessment of DLPNO-MP2 Approximations in Double-Hybrid DFT. *J. Chem. Theory Comput.*, **2023**, 19 (21), 7695–7703. DOI: [10.1021/acs.jctc.3c00896](https://doi.org/10.1021/acs.jctc.3c00896).
- [258] Neese, F.; Schwabe, T.; Grimme, S. *J. Chem. Phys.*, **2007**, 126, 124115.
- [259] Najibi, A.; Casanova-Páez, M.; Goerigk, L. Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. *J. Phys. Chem. A*, **2021**, 125, 4026–4035.
- [260] Schwabe, T.; Grimme, S. *Phys. Chem. Chem. Phys.*, **2006**, 8, 4398.
- [261] Karton, A.; Tarnopolsky, A.; Lamère, J.-F.; Schatz, G. C.; Martin, J. M. L. Highly Accurate First-Principles Benchmark Data Sets for the Parametrization and Validation of Density Functional and Other Approximate Methods. Derivation of a Robust, Generally Applicable, Double-Hybrid Functional for Thermochemistry and Thermochemical Kinetics. *J. Phys. Chem. A*, **2008**, 112, 12868. DOI: [10.1021/jp801805p](https://doi.org/10.1021/jp801805p).
- [262] Tarnopolsky, Alex; Karton, Amir; Sertchook, Rotem; Vuzman, Dana; Martin, Jan M. L. Double-Hybrid Functionals for Thermochemical Kinetics. *J. Phys. Chem. A*, **2008**, 112 (1), 3–8. DOI: [10.1021/jp710179r](https://doi.org/10.1021/jp710179r).
- [263] Yu, Feng. Double-Hybrid Density Functionals Free of Dispersion and Counterpoise Corrections for Non-Covalent Interactions. *J. Phys. Chem. A*, **2014**, 118 (17), 3175–3182. DOI: [10.1021/jp5005506](https://doi.org/10.1021/jp5005506).

- [264] Brémond, Éric; Sancho-García, Juan Carlos; Pérez-Jiménez, Ángel José; Adamo, Carlo. *J. Chem. Phys.*, **2014**, 141, 031101.
- [265] Brémond, Éric; Adamo, Carlo. Seeking for Parameter-Free Double-Hybrid Functionals: The PBE0-DH Model. *J. Chem. Phys.*, **2011**, 135 (2), 024106.
- [266] Casanova-Páez, Marcos; Goerigk, Lars. Time-Dependent Long-Range-Corrected Double-Hybrid Density Functionals with Spin-Component and Spin-Opposite Scaling: A Comprehensive Analysis of Singlet-Singlet and Singlet-Triplet Excitation Energies. *J. Chem. Theory Comput.*, **2021**, 17 (8), 5165–5186. DOI: [10.1021/acs.jctc.1c00535](https://doi.org/10.1021/acs.jctc.1c00535).
- [267] Chai, Jeng-Da; Head-Gordon, Martin. Long-Range Corrected Double-Hybrid Density Functionals. *J. Chem. Phys.*, **2009**, 131 (17), 174105. DOI: [10.1063/1.3244209](https://doi.org/10.1063/1.3244209).
- [268] Brémond, Éric; Savarese, Marika; Pérez-Jiménez, Ángel José; Sancho-García, Juan Carlos; Adamo, Carlo. *J. Chem. Theory Comput.*, **2018**, 14, 4052–4062.
- [269] Brémond, Éric; Pérez-Jiménez, Ángel José; Sancho-García, Juan Carlos; Adamo, Carlo. *J. Chem. Phys.*, **2019**, 150, 201102.
- [270] Casanova-Páez, Marcos; Dardis, Michael B.; Goerigk, Lars. ω B2PLYP & ω B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. *J. Chem. Theory Comput.*, **2019**, 15, 4735. DOI: [10.1021/acs.jctc.9b00013](https://doi.org/10.1021/acs.jctc.9b00013).
- [271] Lehtola, S.; Steigemann, C.; Oliveira, MJT; Marques, MAL. Recent Developments in Libxc – A Comprehensive Library of Functionals for Density Functional Theory. *SoftwareX*, **2019**, 7, 1–5. DOI: [10.1016/j.softx.2017.11.002](https://doi.org/10.1016/j.softx.2017.11.002).
- [272] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.*, **2010**, 132, 154104.
- [273] Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.*, **2011**, 32, 1456.
- [274] Caldeweyher, Eike; Bannwarth, Christoph; Grimme, Stefan. Extension of the D3 Dispersion Coefficient Model. *J. Chem. Phys.*, **2017**, 147 (3), 034112. DOI: [10.1063/1.4993215](https://doi.org/10.1063/1.4993215).
- [275] Vydrov, O. A.; Van Voorhis, T. *J. Chem. Phys.*, **2010**, 133, 244103.
- [276] Hujo, Waldemar; Grimme, Stefan. Performance of Dispersion-Corrected Density Functional Theory for Thermochemistry and Noncovalent Interactions. *J. Chem. Theory Comput.*, **2011**, 7 (12), 3866–3871. DOI: [10.1021/ct200644w](https://doi.org/10.1021/ct200644w).
- [277] Becke, A. D.; Johnson, E. R. A density-functional model of the dispersion interaction. *J. Chem. Phys.*, **2005**, 123, 154101. DOI: [10.1063/1.2065267](https://doi.org/10.1063/1.2065267).
- [278] Johnson, Erin R.; Becke, Axel D. A Post-Hartree–Fock Model of Intermolecular Interactions. *J. Chem. Phys.*, **2005**, 123, 024101. DOI: [10.1063/1.1949201](https://doi.org/10.1063/1.1949201).
- [279] Johnson, Erin R.; Becke, Axel D. A Post-Hartree–Fock Model of Intermolecular Interactions: Inclusion of Higher-Order Corrections. *J. Chem. Phys.*, **2006**, 124, 174104. DOI: [10.1063/1.2190220](https://doi.org/10.1063/1.2190220).
- [280] Grimme, S. *Chem. Eur. J.*, **2012**, 18, 9955–9964.
- [281] Grimme, S. Accurate description of van der Waals complexes by density functional theory including empirical corrections. *J. Comput. Chem.*, **2004**, 25, 1463. DOI: [10.1002/jcc.20078](https://doi.org/10.1002/jcc.20078).
- [282] Lee, K.; Murray, É. D.; Kong, L.; Lundqvist, B. I.; Langreth, D. C. Higher-accuracy van der Waals density functional. *Phys. Rev. B*, **2010**, 82 (8), 081101. DOI: [10.1103/PhysRevB.82.081101](https://doi.org/10.1103/PhysRevB.82.081101).
- [283] Goerigk, L.; Grimme, S. *J. Chem. Theory Comput.*, **2010**, 6, 107.
- [284] Goerigk, L.; Grimme, S. *Phys. Chem. Chem. Phys.*, **2011**, 13, 6670.
- [285] Řezáč, Jan; Riley, Kevin E.; Hobza, Pavel. S66: A Well-balanced Database of Benchmark Interaction Energies Relevant to Biomolecular Structures. *J. Chem. Theory Comput.*, **2011**, 7, 2427–2438. DOI: [10.1021/ct2002946](https://doi.org/10.1021/ct2002946).
- [286] Hujo, W.; Grimme, S. *Phys. Chem. Chem. Phys.*, **2011**, 13, 13942.

- [287] Iron, Mark A.; Janes, Trevor. Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange–Correlation Functionals: The MOBH35 Benchmark Database. *J. Phys. Chem. A*, **2019**, 123 (17), 3761–3781. DOI: [10.1021/acs.jpca.9b01546](https://doi.org/10.1021/acs.jpca.9b01546).
- [288] Jurečka, Petr; Šponer, Jiří; Černý, Jiří; Hobza, Pavel. Benchmark Database of Accurate (MP2 and CCSD(T) Complete Basis Set Limit) Interaction Energies of Small Model Complexes, DNA Base Pairs, and Amino Acid Pairs. *Phys. Chem. Chem. Phys.*, **2006**, 8, 1985–1993. DOI: [10.1039/B600027D](https://doi.org/10.1039/B600027D).
- [289] Arago, Juan; Orti, Enrique; Sancho-Garcia, Juan C. Nonlocal van Der Waals Approach Merged with Double-Hybrid Density Functionals: Toward the Accurate Treatment of Noncovalent Interactions. *J. Chem. Theory Comput.*, **2013**, 9 (8), 3437–3443. DOI: [10.1021/ct4003527](https://doi.org/10.1021/ct4003527).
- [290] Yu, Feng. Spin-Component-Scaled Double-Hybrid Density Functionals with Nonlocal van Der Waals Correlations for Noncovalent Interactions. *J. Chem. Theory Comput.*, **2014**, 10 (10), 4400–4407. DOI: [10.1021/ct500642x](https://doi.org/10.1021/ct500642x).
- [291] Pople, J. A.; Beveridge, D. L. *Approximate Molecular Orbital Theory*. McGraw Hill Inc, **1970**.
- [292] Sedlej, J.; Cooper, I. L. *Semi-Empirical Methods of Quantum Chemistry*. 1985, **John Wiley and Sons**.
- [293] Dewar, M. J. S.; Zebisch, E. G.; Healy, E. F.; Stewart, J. P. *J. Am. Chem. Soc.*, **1985**, 107, 3902.
- [294] Stewart, J. P. *J. Comput. Chem.*, **1989**, 10, 209 & 221.
- [295] Dewar, M. J. S.; Thiel, W. *Theor. Chim. Acta*, **1977**, 46, 89.
- [296] Thiel, W.; Voityuk, A. A. *Theor. Chim. Acta*, **1992**, 81, 391.
- [297] Dewar, M. J. S.; Thiel, W. *J. Am. Chem. Soc.*, **1977**, 99, 4899.
- [298] Pople, J. A.; Segal, G. A. *J. Chem. Phys.*, **1965**, 43, 136.
- [299] Pople, J. A.; Segal, G. A. *J. Chem. Phys.*, **1966**, 44, 3289.
- [300] Santry, D. P. *J. Am. Chem. Soc.*, **1968**, 90, 3309.
- [301] Santry, D. P.; Segal, G. A. *J. Chem. Phys.*, **1967**, 47, 158.
- [302] Pople, J. A.; Beveridge, D. L.; Dobosh, P. A. *J. Chem. Phys.*, **1967**, 47, 2026.
- [303] Clack, D. W.; Hush, N. S.; Yandle, J. R. All-Valence Electron CNDO Calculations on Transition Metal Complexes. *J. Chem. Phys.*, **1972**, 57, 3503. DOI: [10.1063/1.1678785](https://doi.org/10.1063/1.1678785).
- [304] Clack, D. W. INDO MO calculations for first row transition metal complexes. *Mol. Phys.*, **1974**, 27, 1513–1519. DOI: [10.1080/00268977400101281](https://doi.org/10.1080/00268977400101281).
- [305] Clack, D. W.; Smith, W. Clack, D. W., Smith, W. Molecular orbital calculations on transition metal complexes. *Theor. Chim. Acta*, **1974**, 36, 87–92. DOI: [10.1007/BF00554339](https://doi.org/10.1007/BF00554339).
- [306] Böhm, M. C.; Gleiter, R. A CNDO/INDO molecular orbital formalism for the elements H to Br. theory. *Theor. Chim. Acta*, **1981**, 59, 127 & 153. DOI: [10.1007/BF00552536](https://doi.org/10.1007/BF00552536).
- [307] Ridley, J.; Zerner, M. C. *Theor. Chim. Acta*, **1973**, 32, 111.
- [308] Bacon, A. D.; Zerner, M. C. An intermediate neglect of differential overlap theory for transition metal complexes: Fe, Co and Cu chlorides. *Theor. Chim. Acta*, **1979**, 53, 21. DOI: [10.1007/BF00547605](https://doi.org/10.1007/BF00547605).
- [309] Zerner, M. C.; Loew, G. H.; Kirchner, R. F.; Mueller-Westerhoff, U. T. *J. Am. Chem. Soc.*, **1980**, 102, 589.
- [310] Anderson, W. P.; Edwards, W. D.; Zerner, M. C. Calculated spectra of hydrated ions of the first transition-metal series. *Inorg. Chem.*, **1986**, 25, 2728. DOI: [10.1021/ic00236a015](https://doi.org/10.1021/ic00236a015).
- [311] Anderson, W. P.; Cundari, T. R.; Drago, R. S.; Zerner, M. C. Utility of the semiempirical INDO/1 method for the calculation of the geometries of second-row transition-metal species. *Inorg. Chem.*, **1990**, 29, 3. DOI: [10.1021/ic00326a001](https://doi.org/10.1021/ic00326a001).
- [312] Anderson, W. P.; Cundari, T. R.; Zerner, M. C. An intermediate neglect of differential overlap model for second-row transition metal species. *Int. J. Quant. Chem.*, **1991**, 39, 31. DOI: [10.1002/qua.560390106](https://doi.org/10.1002/qua.560390106).
- [313] Zerner, M. C. In Lipkowitz, K. B.; Boyd, D. B., editors, *Reviews in Computational Chemistry*, volume 2, pages 313. Wiley-VCH, **1990**.

- [314] Zerner, M. C. In Salahub, D. R.; Russo, N., editors, *Metal-Ligand Interactions: From Atoms to Clusters to Surfaces*, pages 101. Kluwer Academic Publishers, **1992**.
- [315] Zerner, M. C. In Salahub, D. R.; Russo, N., editors, *Metal-Ligand Interactions: Structure and Reactivity*, pages 493. Kluwer Academic Publishers, **1992**.
- [316] Cory, M. G.; Zerner, M. C. Metal-ligand exchange coupling in transition-metal complexes. *Chem. Rev.*, **1991**, 91, 813. DOI: [10.1021/cr00005a009](https://doi.org/10.1021/cr00005a009).
- [317] Kotzian, M.; Rösch, N.; Zerner, M. C. Intermediate neglect of differential overlap spectroscopic studies on lanthanide complexes. I. Spectroscopic parametrization and application to diatomic lanthanide oxides LnO (Ln=La, Ce, Gd, and Lu). *Theor. Chim. Acta*, **1992**, 81 (3-4), 201–222. DOI: [10.1007/BF01118562](https://doi.org/10.1007/BF01118562).
- [318] Nieke, C.; Reinhold, J. *Theor. Chim. Acta*, **1984**, 65, 99.
- [319] Köhler, H. J.; Birnstock, F. Title not provided. *Z. Chem.*, **1972**, 12 (5), 196.
- [320] Grimme, Stefan; Bannwarth, Christoph; Shushkov, Philip. A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All Spd-Block Elements ($z = 1-86$). *J. Chem. Theory Comput.*, **2017**, 13 (5), 1989–2009. DOI: [10.1021/acs.jctc.7b00118](https://doi.org/10.1021/acs.jctc.7b00118).
- [321] Pracht, Philipp; Caldeweyher, Eike; Ehlert, Sebastian; Grimme, Stefan. A Robust Non-Self-Consistent Tight-Binding Quantum Chemistry Method for Large Molecules. ChemRxiv, **2019**. DOI: [10.26434/chemrxiv.8326202.v1](https://doi.org/10.26434/chemrxiv.8326202.v1).
- [322] Ehlert, Sebastian; Stahn, Marcel; Spicher, Sebastian; Grimme, Stefan. Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. *J. Chem. Theory Comput.*, **2021**, 17 (7), 4250–4261. DOI: [10.1021/acs.jctc.1c00471](https://doi.org/10.1021/acs.jctc.1c00471).
- [323] Cancès, E.; Maday, Y.; Stamm, B. Domain decomposition for implicit solvation models. *J. Chem. Phys.*, **2013**, 139, 054111. DOI: [10.1063/1.4816767](https://doi.org/10.1063/1.4816767).
- [324] Neugebauer, Hagen; Bädorf, Benedikt; Ehlert, Sebastian; Hansen, Andreas; Grimme, Stefan. High-throughput screening of spin states for transition metal complexes with spin-polarized extended tight-binding methods. *J. Comput. Chem.*, **2023**, 44 (27), 2120–2129. DOI: <https://doi.org/10.1002/jcc.27185>.
- [325] Sure, R.; Grimme, S. *J. Comput. Chem.*, **2013**, 34, 1672–1685.
- [326] Brandenburg, J. G.; Bannwarth, C.; Hansen, A.; Grimme, S. B97-3c: A Revised Low-Cost Variant of the B97-D Density Functional Method. *J. Chem. Phys.*, **2018**, 148 (6), 064104.
- [327] Ehlert, Sebastian; Huniar, Uwe; Ning, Jinliang; Furness, James W.; Sun, Jianwei; Kaplan, Aaron D.; Perdew, John P.; Brandenburg, Jan Gerit. r²SCAN-D4: Dispersion Corrected Meta-Generalized Gradient Approximation for General Chemical Applications. *J. Chem. Phys.*, **2021**, 154 (6), 061101. arXiv:[10.1063/5.0041008](https://arxiv.org/abs/10.1063/5.0041008), DOI: [10.1063/5.0041008](https://doi.org/10.1063/5.0041008).
- [328] Langreth, D.C.; Perdew, J.P. The exchange-correlation energy of a metallic surface. *Solid State Communications*, **1975**, 17 (11), 1425–1429. DOI: [10.1016/0038-1098\(75\)90618-3](https://doi.org/10.1016/0038-1098(75)90618-3).
- [329] Furche, Philipp. Molecular tests of the random phase approximation to the exchange-correlation energy functional. *Phys. Rev. B*, **2001**, 64, 195120. DOI: [10.1103/PhysRevB.64.195120](https://doi.org/10.1103/PhysRevB.64.195120).
- [330] Furche, Philipp. Developing the random phase approximation into a practical post-Kohn–Sham correlation model. *The Journal of Chemical Physics*, **2008**, 129 (11), 114105. arXiv:https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/1.2977789/13579843/114105_1_online.pdf, DOI: [10.1063/1.2977789](https://doi.org/10.1063/1.2977789).
- [331] Trushin, Egor; Thierbach, Adrian; Görling, Andreas. Toward chemical accuracy at low computational cost: Density-functional theory with σ -functionals for the correlation energy. *The Journal of Chemical Physics*, **2021**, 154 (1), 014104. arXiv:https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/5.0026849/15583499/014104_1_online.pdf, DOI: [10.1063/5.0026849](https://doi.org/10.1063/5.0026849).
- [332] Lochan, Rohini C.; Head-Gordon, Martin. Orbital-Optimized Opposite-Spin Scaled Second-Order Correlation: An Economical Method to Improve the Description of Open-Shell Molecules. *J. Chem. Phys.*, **2007**, 126 (16), 164101. DOI: [10.1063/1.2718952](https://doi.org/10.1063/1.2718952).
- [333] McWeeny, R. *Methods of Molecular Quantum Mechanics. 2nd Edition*. Academic Press, **1992**.

- [334] Cremer, D. In Schleyer, P. v. R., editor, *Encyclopedia of Computational Chemistry*, pages 1706. John Wiley and Sons, **1998**.
- [335] Saebo, S.; Almlöf, J. *Chem. Phys. Lett.*, **1989**, 154, 83.
- [336] Head-Gordon, M.; Pople, J. A. *Chem. Phys. Lett.*, **1988**, 153, 503.
- [337] Lauderdale, W. J.; Stanton, J. F.; Gauss, J.; Watts, J. D.; Bartlett, R. J. Many-body perturbation theory with a restricted open-shell Hartree–Fock reference. *Chem. Phys. Lett.*, **1991**, 187 (1-2), 21–28. DOI: [10.1016/0009-2614\(91\)90478-R](https://doi.org/10.1016/0009-2614(91)90478-R).
- [338] Knowles, Peter J.; Andrews, James S.; Amos, Roger D.; Handy, Nicholas C.; Pople, John A. Restricted Møller–Plesset Theory for Open-Shell Molecules. *Chem. Phys. Lett.*, **1991**, 186 (2-3), 130–136. DOI: [10.1016/0009-2614\(91\)85118-G](https://doi.org/10.1016/0009-2614(91)85118-G).
- [339] Pople, J. A.; Binkley, J. S.; Seeger, R. *Int. J. Quant. Chem. Symp.*, **1976**, 10, 1.
- [340] Krishnan, R.; Frisch, M. J.; Pople, J. A. Contribution of triple substitutions to the electron correlation energy in fourth order perturbation theory. *J. Chem. Phys.*, **1980**, 72 (7), 4244–4245. DOI: [10.1063/1.439657](https://doi.org/10.1063/1.439657).
- [341] Handy, N. C.; Knowles, P. J.; Somasundram, K. *Theor. Chem. Acc.*, **1985**, 68, 87.
- [342] Weigend, F.; Häser, M.; Patzelt, H.; Ahlrichs, R. *Chem. Phys. Lett.*, **1998**, 294, 143.
- [343] Weigend, F.; Häser, M. *Theor. Chem. Acc.*, **1997**, 97, 331.
- [344] Feyereisen, M.; Fitzgerald, G.; Komornicki, A. *Chem. Phys. Lett.*, **1993**, 208, 359.
- [345] Bernholdt, D. E.; Harrison, R. J. Large-scale correlated electronic structure calculations: the RI-MP2 method on parallel computers. *Chem. Phys. Lett.*, **1996**, 250, 477. DOI: [10.1016/0009-2614\(96\)00054-1](https://doi.org/10.1016/0009-2614(96)00054-1).
- [346] Grimme, S. *J. Chem. Phys.*, **2003**, 118, 9095–9102.
- [347] Stoychev, Georgi L.; Auer, Alexander A.; Neese, Frank. Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory. *J. Chem. Theory Comput.*, **2018**, 14 (9), 4756–4771. DOI: [10.1021/acs.jctc.8b00624](https://doi.org/10.1021/acs.jctc.8b00624).
- [348] Tran, Van Anh; Neese, Frank. Double-Hybrid Density Functional Theory for g-Tensor Calculations Using Gauge Including Atomic Orbitals. *J. Chem. Phys.*, **2020**, 153 (5), 054105. DOI: [10.1063/5.0013799](https://doi.org/10.1063/5.0013799).
- [349] Pinski, P.; Riplinger, C.; Valeev, E. F.; Neese, Frank. *J. Chem. Phys.*, **2015**, 143, 034108.
- [350] Pavošević, F.; Pinski, P.; Riplinger, C.; Neese, F.; Valeev, E.F. SparseMaps – A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. *J. Chem. Phys.*, **2016**, 144, 144109.
- [351] Pinski, Peter; Neese, Frank. Communication: Exact Analytical Derivatives for the Domain-Based Local Pair Natural Orbital MP2 Method (DLPNO-MP2). *J. Chem. Phys.*, **2018**, 148, 031101. DOI: [10.1063/1.5011204](https://doi.org/10.1063/1.5011204).
- [352] Pinski, Peter; Neese, Frank. Analytical Gradient for the Domain-Based Local Pair Natural Orbital Second Order Møller–Plesset Perturbation Theory Method (DLPNO-MP2). *J. Chem. Phys.*, **2019**, 150, 164102.
- [353] Scheurer, P.; Schwarz, W. H. E. Continuous Degeneracy of Sets of Localized Orbitals. *Int. J. Quantum Chem.*, **2000**, 76, 428–433.
- [354] Stoychev, Georgi L.; Auer, Alexander A.; Gauss, Jürgen; Neese, Frank. DLPNO-MP2 Second Derivatives for the Computation of Polarizabilities and NMR Shieldings. *J. Chem. Phys.*, **2021**, 154 (16), 164110. DOI: [10.1063/5.0047125](https://doi.org/10.1063/5.0047125).
- [355] Sparta, Manuel; Retegan, Marius; Pinski, Peter; Riplinger, Christoph; Becker, Ute; Neese, Frank. Multilevel Approaches within the Local Pair Natural Orbital Framework. *J. Chem. Theory Comput.*, **2017**, 13 (7), 3198–3207. DOI: [10.1021/acs.jctc.7b00260](https://doi.org/10.1021/acs.jctc.7b00260).
- [356] Jensen, F. *Introduction to Computational Chemistry*. Wiley, **1999**.
- [357] Koch, W.; Holthausen, M. C. *A Chemist’s Guide to Density Functional Theory*. Wiley-VCH, **2000**.
- [358] Neese, F.; Schwabe, T.; Kossmann, S.; Schirmer, B.; Grimme, S. *J. Chem. Theory Comput.*, **2009**, 5, 3060.

- [359] Shee, James; Loipersberger, Matthias; Rettig, Adam; Lee, Joonho; Head-Gordon, Martin. Regularized Second-Order Møller–Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost. *J. Phys. Chem. Lett.*, **2021**, 12 (50), 12084–12097. DOI: [10.1021/acs.jpcclett.1c03468](https://doi.org/10.1021/acs.jpcclett.1c03468).
- [360] Neese, F. Importance of Direct Spin-Spin Coupling and Spin-Flip Excitations for the Zero-Field Splittings of Transition Metal Complexes: A Case Study. *J. Am. Chem. Soc.*, **2006**, 128, 10213.
- [361] Krupička, Martin; Sivalingam, Kantharuban; Huntington, Lee; Auer, Alexander A.; Neese, Frank. A toolchain for the automatic generation of computer codes for correlated wavefunction calculations. *J. Comput. Chem.*, **2017**, 38 (21), 1853–1868. DOI: [10.1002/jcc.24833](https://doi.org/10.1002/jcc.24833).
- [362] Lechner, M. H.; Papadopoulos, A.; Sivalingam, K.; Auer, A. A.; Kosłowski, A.; Becker, U.; Wennmohs, F.; Neese, F. Code generation in ORCA: Progress, Efficiency and Tight integration. *Phys. Chem. Chem. Phys.*, **2024**, 26 (21), 15205–15220.
- [363] Parr, R. G. *Density Functional Theory of Atoms and Molecules*. International Series of Monographs on Chemistry. Oxford University Press, **1994**. ISBN 978-0-19-509276-9.
- [364] Ahlrichs, R. Many body perturbation calculations and coupled electron pair models. *Comp. Phys. Comm.*, **1979**, 17, 31. DOI: [10.1016/0010-4655\(79\)90067-5](https://doi.org/10.1016/0010-4655(79)90067-5).
- [365] Gdanitz, R. J. *Int. J. Quant. Chem.*, **2001**, 85, 281.
- [366] Gdanitz, R. J.; Ahlrichs, R. *Chem. Phys. Lett.*, **0143**, 1988, 413.
- [367] Szalay, P. G.; Bartlett, R. J. *Chem. Phys. Lett.*, **1993**, 214, 481.
- [368] Ahlrichs, R.; Scharf, P.; Ehrhardt, C. The coupled pair functional (CPF). A size consistent modification of the CI(SD) based on an energy functional. *J. Chem. Phys.*, **1985**, 82, 890. DOI: [10.1063/1.448517](https://doi.org/10.1063/1.448517).
- [369] Kollmar, Christian; Neese, Frank. The coupled electron pair approximation: Variational formulation and spin adaptation. *Mol. Phys.*, **2010**, 108 (19-20), 2449–2458. DOI: [10.1080/00268976.2010.496743](https://doi.org/10.1080/00268976.2010.496743).
- [370] Kollmar, Christian; Neese, Frank. The relationship between double excitation amplitudes and Z vector components in some post-Hartree-Fock correlation methods. *J. Chem. Phys.*, **2011**, 135 (6), 064103. DOI: [10.1063/1.3618720](https://doi.org/10.1063/1.3618720).
- [371] Chong, D. P.; Langhoff, S. R. A modified coupled pair functional approach. *J. Chem. Phys.*, **1986**, 84, 5606–5610. DOI: [10.1063/1.449920](https://doi.org/10.1063/1.449920).
- [372] Scuseria, G. E.; III, H. F. Schaefer. *Chem. Phys. Lett.*, **1987**, 142, 354.
- [373] Handy, N. C.; Pople, J. A.; Head-Gordon, M.; Raghavachari, K.; Trucks, G. W. *Chem. Phys. Lett.*, **1989**, 164, 185.
- [374] Kollmar, Christian; Hesselmann, Andreas. The role of orbital transformations in coupled-pair functionals. *Theor. Chem. Acc.*, **2010**, 127 (5-6), 311–320. DOI: [10.1007/s00214-010-0846-z](https://doi.org/10.1007/s00214-010-0846-z).
- [375] Salter, E. A.; Trucks, G. W.; Bartlett, R. J. *J. Chem. Phys.*, **1989**, 90, 1752.
- [376] Kollmar, Christian; Neese, Frank. An orbital-invariant and strictly size extensive post-Hartree-Fock correlation functional. *J. Chem. Phys.*, **2011**, 135 (8), 084102. DOI: [10.1063/1.3624567](https://doi.org/10.1063/1.3624567).
- [377] Huntington, L. M. J.; Nooijen, M. *J. Chem. Phys.*, **2010**, 133, 184109.
- [378] Huntington, Lee M. J.; Hansen, Andreas; Neese, Frank; Nooijen, Marcel. Accurate Thermochemistry from a Parameterized Coupled-Cluster Singles and Doubles Model and a Local Pair Natural Orbital Based Implementation for Applications to Larger Systems. *J. Chem. Phys.*, **2012**, 136, 064101. DOI: [10.1063/1.3682325](https://doi.org/10.1063/1.3682325).
- [379] Pulay, P.; Saebo, S.; Meyer, W. *J. Chem. Phys.*, **1984**, 81, 1901.
- [380] Hampel, C.; Peterson, K. A.; Werner, H. J. *Chem. Phys. Lett.*, **1992**, 190, 1.
- [381] Scuseria, G. E.; Janssen, C. L.; III, H. F. Schaefer. *J. Chem. Phys.*, **1988**, 89, 7382.
- [382] Heully, J. L.; Malrieu, J.-P. *J. Mol. Struct.: THEOCHEM*, **2006**, 768, 53.
- [383] Neese, F.; Hansen, A.; Liakos, D. G. *J. Chem. Phys.*, **2009**, 131, 064103.
- [384] Hansen, A.; Liakos, D. G.; Neese, F. *J. Chem. Phys.*, **2011**, 135, 214102.

- [385] Neese, F.; Hansen, A.; Wennmohs, F.; Grimme, S. *Acc. Chem. Res.*, **2009**, 42, 641.
- [386] Neese, F.; Liakos, D. G.; Ye, S. F. *J. Biol. Inorg. Chem.*, **2011**, 16, 821.
- [387] Semidalas, Emmanouil; Martin, Jan M. L. Automatic generation of complementary auxiliary basis sets for explicitly correlated methods. *J. Comput. Chem.*, **2022**, 43 (25), 1690–1700. DOI: [10.1002/jcc.26970](https://doi.org/10.1002/jcc.26970).
- [388] Liakos, Dimitrios G.; Izsák, Róbert; Valeev, Edward F.; Neese, Frank. What is the most efficient way to reach the canonical MP2 basis set limit? *Mol. Phys.*, **2013**, 111 (19-20), 2653–2662. DOI: [10.1080/00268976.2013.811812](https://doi.org/10.1080/00268976.2013.811812).
- [389] Liakos, D. G.; Neese, F. Improved correlation energy extrapolation schemes based on local pair natural orbital methods. *J. Phys. Chem. A*, **2012**, 116 (19), 4801–4816. DOI: [10.1021/jp300997x](https://doi.org/10.1021/jp300997x).
- [390] Li, S.; Ma, J.; Jiang, Y. Linear Scaling Local Correlation Approach for Solving the Coupled Cluster Equations of Large Systems. *J. Comput. Chem.*, **2002**, 23, 237–244. DOI: [10.1002/jcc.10003](https://doi.org/10.1002/jcc.10003).
- [391] Li, S.; Shen, J.; Li, W.; Jiang, Y. An Efficient Implementation of the “Cluster-in-Molecule” Approach for Local Electron Correlation Calculations. *J. Chem. Phys.*, **2006**, 125, 074109. DOI: [10.1063/1.2244566](https://doi.org/10.1063/1.2244566).
- [392] Li, W.; Piecuch, P.; Gour, J.; Li, S. Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Approaches. *J. Chem. Phys.*, **2009**, 131, 114109. DOI: [10.1063/1.3218842](https://doi.org/10.1063/1.3218842).
- [393] Rolik, Z.; Kallay, M. A General-Order Local Coupled-Cluster Method Based on the Cluster-in-Molecule Approach. *J. Chem. Phys.*, **2011**, 135, 104111. DOI: [10.1063/1.3632085](https://doi.org/10.1063/1.3632085).
- [394] Guo, Y.; Li, W.; Li, S. Improved Cluster-in-Molecule Local Correlation Approach for Electron Correlation Calculation of Large Systems. *J. Phys. Chem. A*, **2014**, 118 (39), 8996–9004. DOI: [10.1021/jp501976x](https://doi.org/10.1021/jp501976x).
- [395] Guo, Yang; Becker, Ute; Neese, Frank. Comparison and Combination of “Direct” and Fragment Based Local Correlation Methods: Cluster in Molecules and Domain Based Local Pair Natural Orbital Perturbation and Coupled Cluster Theories. *J. Chem. Phys.*, **2018**, 148 (12), 124117. DOI: [10.1063/1.5021898](https://doi.org/10.1063/1.5021898).
- [396] Förner, W.; Ladik, J.; Otto, P.; Čížek, J. Coupled-Cluster Studies. II. The Role of Localization in Correlation Calculations on Extended Systems. *Chem. Phys.*, **1985**, 97, 251–262. DOI: [10.1016/0301-0104\(85\)87035-X](https://doi.org/10.1016/0301-0104(85)87035-X).
- [397] Riplinger, C.; Neese, F. *J. Chem. Phys.*, **2013**, 138, 034106.
- [398] Neese, F.; Wennmohs, F.; Hansen, A. *J. Chem. Phys.*, **2009**, 130, 114108.
- [399] Liakos, Dimitrios G.; Hansen, Andreas; Neese, Frank. Weak molecular interactions studied with parallel implementations of the local pair natural orbital coupled pair and coupled cluster methods. *J. Chem. Theory Comput.*, **2011**, 7 (1), 76–87. DOI: [10.1021/ct100529u](https://doi.org/10.1021/ct100529u).
- [400] Riplinger, C.; Sandhoefer, B.; Hansen, A.; Neese, F. *J. Chem. Phys.*, **2013**, 139, 134101.
- [401] Riplinger, C.; Pinski, P.; Becker, U.; Valeev, E. F.; Neese, Frank. *J. Chem. Phys.*, **2016**, 144, 024109.
- [402] Datta, D.; Kossmann, S.; Neese, F. Analytic energy derivatives for the calculation of the first-order molecular properties using the domain-based local pair-natural orbital coupled-cluster theory. *J. Chem. Phys.*, **2016**, 175, 114101. DOI: [10.1063/1.4962369](https://doi.org/10.1063/1.4962369).
- [403] Saitow, M.; Becker, U.; Riplinger, C.; Valeev, E. F.; Neese, F. *J. Chem. Phys.*, **2017**, 146, 164105.
- [404] Guo, Yang; Riplinger, Christoph; Becker, Ute; Liakos, Dimitrios G.; Minenkov, Yury; Cavallo, Luigi; Neese, Frank. Communication: An Improved Linear Scaling Perturbative Triples Correction for the Domain Based Local Pair-Natural Orbital Based Singles and Doubles Coupled Cluster Method [DLPNO-CCSD(T)]. *J. Chem. Phys.*, **2018**, 148 (1), 011101. DOI: [10.1063/1.5011798](https://doi.org/10.1063/1.5011798).
- [405] Schütz, M.; Werner, H. J. *Chem. Phys. Lett.*, **2000**, 318, 370.
- [406] Schütz, M.; Werner, H. J. *J. Chem. Phys.*, **2001**, 114, 661.
- [407] Schütz, Martin; Manby, Frederick R. Linear scaling local coupled cluster theory with density fitting. Part I: 4-external integrals. *Phys. Chem. Chem. Phys.*, **2003**, 5 (16), 3349–3358.
- [408] Schütz, Martin. A new, fast, semi-direct implementation of linear scaling local coupled cluster theory. *Phys. Chem. Chem. Phys.*, **2002**, 4 (16), 3941–3947.

- [409] Meyer, Wilfried. Ionization energies of water from PNO-CI calculations. *Int. J. Quantum Chem.*, **1971**, 5 (S5), 341–348.
- [410] Ahlrichs, R.; Lischka, H.; Staemmler, V.; Kutzelnigg, W. PNO–CI (pair natural orbital configuration interaction) and CEPA–PNO (coupled electron pair approximation with pair natural orbitals) calculations of molecular systems. I. Outline of the method for closed-shell states. *J. Chem. Phys.*, **1975**, 62 (4), 1225–1234.
- [411] Meyer, Wilfried. PNO–CI Studies of electron correlation effects. I. Configuration expansion by means of nonorthogonal orbitals, and application to the ground state and ionized states of methane. *J. Chem. Phys.*, **1973**, 58 (3), 1017–1035.
- [412] Werner, Hans-Joachim; Meyer, Wilfried. PNO-CI and PNO-CEPA studies of electron correlation effects: V. Static dipole polarizabilities of small molecules. *Mol. Phys.*, **1976**, 31 (3), 855–872.
- [413] Liakos, Dimitrios G.; Sparta, Manuel; Kesharwani, Manoj K.; Martin, Jan M. L.; Neese, Frank. Exploring the Accuracy Limits of Local Pair Natural Orbital Coupled-Cluster Theory. *J. Chem. Theory Comput.*, **2015**, 11 (4), 1525–1539. DOI: [10.1021/acs.jctc.5b00078](https://doi.org/10.1021/acs.jctc.5b00078).
- [414] Altun, Ahmet; Riplinger, Christoph; Neese, Frank; Bistoni, Giovanni. Exploring the Accuracy Limits of PNO-Based Local Coupled-Cluster Calculations for Transition-Metal Complexes. *J. Chem. Theory Comput.*, **2023**, 19 (7), 2039–2047.
- [415] Lee, T. J.; Taylor, P. R. A diagnostic for determining the quality of single-reference electron correlation methods. *Int. J. Quant. Chem. Symp.*, **1989**, 23, 199–207. DOI: [10.1002/qua.560360824](https://doi.org/10.1002/qua.560360824).
- [416] Wennmohs, F.; Neese, F. *Chem. Phys.*, **2008**, 343, 217–230. DOI: .
- [417] Ahlrichs, R.; Scharf, P. The Coupled Pair Approximation. In Lawley, K. P., editor, *Advances in Chemical Physics: Ab Initio Methods in Quantum Chemistry, Part I*, Advances in Chemical Physics, pages 1–42. Wiley, **1987**.
- [418] Siegbahn, Per E. M. Direct Configuration Interaction with a Reference State Composed of Many Reference Configurations. *Int. J. Quant. Chem.*, **1980**, 18 (5), 1229–1242. DOI: [10.1002/qua.560180510](https://doi.org/10.1002/qua.560180510).
- [419] Meyer, Wilfried. Configuration Expansion by Means of Pseudonatural Orbitals. In Schaefer III, Henry F., editor, *Methods of Electronic Structure Theory*, pages 413–446. Springer US, **1977**.
- [420] Sivalingam, K.; Krupicka, M.; Auer, A. A.; Neese, F. Comparison of fully internally and strongly contracted multireference configuration interaction procedures. *J. Chem. Phys.*, **2016**, 145, 054104. DOI: [10.1063/1.4950161](https://doi.org/10.1063/1.4950161).
- [421] Saitow, Masaaki; Kurashige, Yuki; Yanai, Takeshi. Multireference Configuration Interaction Theory Using Cumulant Reconstruction with Internal Contraction of Density Matrix Renormalization Group Wave Function. *J. Chem. Phys.*, **2013**, 139, 044118. DOI: [10.1063/1.4816627](https://doi.org/10.1063/1.4816627).
- [422] Guo, Yang; Sivalingam, Kantharuban; Neese, Frank. Approximations of Density Matrices in N-Electron Valence State Second-Order Perturbation Theory (NEVPT2). I. Revisiting the NEVPT2 Construction. *J. Chem. Phys.*, **2021**, 154 (21), 214111. DOI: [10.1063/5.0051211](https://doi.org/10.1063/5.0051211).
- [423] Lyakh, Dmitry I.; Musiał, Monika; Lotrich, Victor F.; Bartlett, Rodney J. Multireference Nature of Chemistry: The Coupled-Cluster View. *Chem. Rev.*, **2012**, 112 (1), 182–243. DOI: [10.1021/cr2001417](https://doi.org/10.1021/cr2001417).
- [424] Evangelista, Francesco A.; Gauss, Jürgen. An Orbital-Invariant Internally Contracted Multireference Coupled Cluster Approach. *J. Chem. Phys.*, **2011**, 134 (11), 114102. DOI: [10.1063/1.3559149](https://doi.org/10.1063/1.3559149).
- [425] Hanauer, Matthias; Köhn, Andreas. Pilot Applications of Internally Contracted Multireference Coupled Cluster Theory, and How to Choose the Cluster Operator Properly. *J. Chem. Phys.*, **2011**, 134 (20), 204111. DOI: [10.1063/1.3592786](https://doi.org/10.1063/1.3592786).
- [426] Jankowski, K.; Paldus, J. Applicability of Coupled-Pair Theories to Quasidegenerate Electronic States: A Model Study. *Int. J. Quantum Chem.*, **1980**, 18 (5), 1243–1269. DOI: [10.1002/qua.560180511](https://doi.org/10.1002/qua.560180511).
- [427] Guo, Yang; Sivalingam, Kantharuban; Kollmar, Christian; Neese, Frank. Approximations of Density Matrices in N-Electron Valence State Second-Order Perturbation Theory (NEVPT2). II. The Full Rank NEVPT2 (FR-NEVPT2) Formulation. *J. Chem. Phys.*, **2021**, 154 (21), 214113. DOI: [10.1063/5.0051218](https://doi.org/10.1063/5.0051218).

- [428] Angeli, Celestino; Bories, Benoît; Cavallini, Alex; Cimiraglia, Renzo. Third-order multireference perturbation theory: The n-electron valence state perturbation-theory approach. *J. Chem. Phys.*, **2006**, 124 (5), 054108. DOI: [10.1063/1.2148946](https://doi.org/10.1063/1.2148946).
- [429] Kempfer, Emily M.; Sivalingam, Kantharuban; Neese, Frank. Efficient Implementation of Approximate Fourth Order N-Electron Valence State Perturbation Theory. *J. Chem. Theory Comput.*, **2025**, 21 (8), 3953–3967. DOI: [10.1021/acs.jctc.4c01735](https://doi.org/10.1021/acs.jctc.4c01735).
- [430] Kollmar, Christian; Sivalingam, Kantharuban; Helmich-Paris, Benjamin; Angeli, Celestino; Neese, Frank. A perturbation-based super-CI approach for the orbital optimization of a CASSCF wave function. *J. Comput. Chem.*, **2019**, 40 (14), 1463–1470. DOI: [10.1002/jcc.25801](https://doi.org/10.1002/jcc.25801).
- [431] Helmich-Paris, Benjamin. A trust-region augmented Hessian implementation for state-specific and state-averaged CASSCF wave functions. *J. Chem. Phys.*, **2022**, 156 (20), 204104. Publisher: American Institute of Physics. DOI: [10.1063/5.0090447](https://doi.org/10.1063/5.0090447).
- [432] Lang, Lucas; Neese, Frank. Spin-Dependent Properties in the Framework of the Dynamic Correlation Dressed Complete Active Space Method. *J. Chem. Phys.*, **2019**, 150 (10), 104104. DOI: [10.1063/1.5085203](https://doi.org/10.1063/1.5085203).
- [433] Atanasov, Mihail; Ganyushin, Dmitry; Sivalingam, Kantharuban; Neese, Frank. A Modern First-Principles View on Ligand Field Theory Through the Eyes of Correlated Multireference Wavefunctions. In Mingos, David Michael P.; Day, Peter; Dahl, Jens Peder, editors, *Molecular Electronic Structures of Transition Metal Complexes II*, number 143 in Structure and Bonding, pages 149–220. Springer Berlin Heidelberg, **2011**. DOI: [10.1007/430_2011_57](https://doi.org/10.1007/430_2011_57).
- [434] Lang, Lucas; Atanasov, Mihail; Neese, Frank. Improvement of Ab Initio Ligand Field Theory by Means of Multistate Perturbation Theory. *J. Phys. Chem. A*, **2020**, 124 (5), 1025–1037. DOI: [10.1021/acs.jpca.9b11227](https://doi.org/10.1021/acs.jpca.9b11227).
- [435] Atanasov, Mihail; Ganyushin, Dmitry; Pantazis, Dimitrios A.; Sivalingam, Kantharuban; Neese, Frank. Detailed Ab Initio First-Principles Study of the Magnetic Anisotropy in a Family of Trigonal Pyramidal Iron(II) Pyrrolide Complexes. *Inorg. Chem.*, **2011**, 50 (16), 7460–7477. DOI: [10.1021/ic200196k](https://doi.org/10.1021/ic200196k).
- [436] Suturina, Elizaveta A.; Maganas, Dimitrios; Bill, Eckhard; Atanasov, Mihail; Neese, Frank. Magneto-Structural Correlations in a Series of Pseudotetrahedral [CoII(XR)4]2– Single Molecule Magnets: An Ab Initio Ligand Field Study. *Inorg. Chem.*, **2015**, 54 (20), 9948–9961. DOI: [10.1021/acs.inorgchem.5b01706](https://doi.org/10.1021/acs.inorgchem.5b01706).
- [437] Aravena, Daniel; Atanasov, Mihail; Neese, Frank. Periodic Trends in Lanthanide Compounds through the Eyes of Multireference Ab Initio Theory. *Inorg. Chem.*, **2016**, 55 (9), 4457–4469. DOI: [10.1021/acs.inorgchem.6b00244](https://doi.org/10.1021/acs.inorgchem.6b00244).
- [438] Jung, Julie; Atanasov, Mihail; Neese, Frank. Ab Initio Ligand-Field Theory Analysis and Covalency Trends in Actinide and Lanthanide Free Ions and Octahedral Complexes. *Inorg. Chem.*, **2017**, 56 (15), 8802–8816. DOI: [10.1021/acs.inorgchem.7b00642](https://doi.org/10.1021/acs.inorgchem.7b00642).
- [439] Singh, Saurabh Kumar; Eng, Julien; Atanasov, Mihail; Neese, Frank. Covalency and Chemical Bonding in Transition Metal Complexes: An Ab Initio Based Ligand Field Perspective. *Coordin. Chem. Rev.*, **2017**, 344, 2–25. DOI: [10.1016/j.ccr.2017.03.018](https://doi.org/10.1016/j.ccr.2017.03.018).
- [440] Chakraborty, Uttam; Demeshko, Serhiy; Meyer, Franc; Rebreyend, Christophe; de Bruin, Bas; Atanasov, Mihail; Neese, Frank; Mühldorf, Bernd; Wolf, Robert. Electronic Structure and Magnetic Anisotropy of an Unsaturated Cyclopentadienyl Iron(I) Complex with 15 Valence Electrons. *Angew. Chem. Int. Ed.*, **2017**, 56 (27), 7995–7999. DOI: [10.1002/anie.201702454](https://doi.org/10.1002/anie.201702454).
- [441] Chilkuri, Vijay Gopal; DeBeer, Serena; Neese, Frank. Revisiting the Electronic Structure of FeS Monomers Using Ab Initio Ligand Field Theory and the Angular Overlap Model. *Inorg. Chem.*, **2017**, 56 (17), 10418–10436. DOI: [10.1021/acs.inorgchem.7b01371](https://doi.org/10.1021/acs.inorgchem.7b01371).
- [442] Chilkuri, Vijay Gopal; DeBeer, Serena; Neese, Frank. Ligand Field Theory and Angular Overlap Model Based Analysis of the Electronic Structure of Homovalent Iron–Sulfur Dimers. *Inorg. Chem.*, **2020**, 59 (2), 984–995. DOI: [10.1021/acs.inorgchem.9b00974](https://doi.org/10.1021/acs.inorgchem.9b00974).
- [443] Chilkuri, Vijay Gopal; Neese, Frank. Comparison of Many-Particle Representations for Selected-CI I: A Tree Based Approach. *J. Comput. Chem.*, **2021**, 42 (14), 982–1005. DOI: [10.1002/jcc.26518](https://doi.org/10.1002/jcc.26518).