

COMPLETE LIST OF PUBLICATIONS

A. Peer reviewed publications

1. S. Coriani, P. Lazzeretti, M. Malagoli, and R. Zanasi. "On CHF calculations of second-order magnetic properties using the method of continuous transformation of origin of the current density". *Theor. Chim. Acta* **89** (1994) 181-192
2. S. Coriani, A. Rizzo, K. Ruud, and T. Helgaker. "MCSCF calculations of hyperpolarizabilities and nuclear shielding polarizabilities of CO and CH₄". *Mol. Phys.* **88** (1996) 931-947
3. S. Coriani, A. Rizzo, K. Ruud, and T. Helgaker. "Cotton-Mouton effect and shielding polarizabilities of ethylene: an MCSCF study". *Chem. Phys.* **216** (1997) 53-66
4. K. Ruud, T. Helgaker, A. Rizzo, S. Coriani, K.V. Mikkelsen. "The Cotton-Mouton Effect (CME) of liquid water. Part I: the dielectric continuum model". *J. Chem. Phys.* **107** (1997) 894-901
5. K. Ruud, H. Ågren, P. Dahle, T. Helgaker, A. Rizzo, S. Coriani, H. Koch, K. Sylvester-Hvid, and K.V. Mikkelsen. "The Cotton-Mouton Effect (CME) of liquid water. Part II: the semi-continuum model". *J. Chem. Phys.* **108** (1998) 599-603
6. S. Coriani, C. Hättig, P. Jørgensen, A. Halkier, and A. Rizzo. "Coupled Cluster calculations of Verdet Constants". *Chem. Phys. Lett.* **281** (1997) 445-451; *ibidem* **293** (1998) 324 (erratum).
7. S. Coriani, M. Jaszunski, A. Rizzo and K. Ruud. "MCSCF nuclear spin-rotation constants of ¹⁷O in ¹⁶O¹⁷O¹⁶O and ¹⁷O¹⁶O¹⁶O". *Chem. Phys. Lett.* **287** (1998) 677-681.
8. B. Fernandez, S. Coriani, and A. Rizzo. "MCSCF polarizability and hyperpolarizabilities of HCl and HBr". *Chem. Phys. Lett.* **288** (1998) 677-688
9. S. Coriani, C. Hättig, P. Jørgensen, A. Rizzo and K. Ruud. "Coupled cluster investigation of the electric field gradient induced birefringence of H₂, N₂, C₂H₂ and CH₄". *J. Chem. Phys.* **109** (1998) 7176-7184
10. A. Halkier, S. Coriani, and P. Jørgensen. "The molecular electric quadrupole moment of N₂". *Chem. Phys. Lett.* **294** (1998) 292-296
11. C. Hättig, O. Christiansen, S. Coriani, and P. Jørgensen. "Static and frequency-dependent polarizabilities of excited singlet states using coupled cluster response theory". *J. Chem. Phys.* **109** (1998) 9237-9243
12. S. Coriani, P. Jørgensen, A. Rizzo, K. Ruud, and J. Olsen. "Ab initio determinations of Magnetic Circular Dichroism". *Chem. Phys. Lett.* **300** (1999) 61
13. A. Halkier and S. Coriani. "On the molecular electric quadrupole moment of C₂H₂". *Chem. Phys. Lett.* **303** (1999) 408-412
14. S. Coriani, C. Hättig, A. Rizzo, P. Jørgensen. "The electric-field-gradient-induced birefringence of He, Ne, Ar and SF₆". *J. Chem. Phys.* **111** (1999) 7828-7836
15. S. Coriani, C. Hättig, P. Jørgensen, T. Helgaker. "Gauge-origin independent magneto optical activity within coupled-cluster response theory". *J. Chem. Phys.* **113** (2000) 3561-3572
16. A. Rizzo, S. Coriani, A. Halkier, C. Hättig. "On the electric-field-gradient-induced birefringence of a polar molecule: CO". *J. Chem. Phys.* **113** (2000) 3077-3087
17. S. Coriani, A. Halkier, P. Jørgensen, A. Rizzo, J. Gauss, and O. Christiansen. "Coupled Cluster investigation of Sternheimer shieldings and nuclear electric field gradient polarizabilities". *J. Chem. Phys.* **113** (2000) 1688-1697
18. S. Coriani, A. Halkier, A. Rizzo, and K. Ruud. "On the molecular electric quadrupole moment and electric-field-gradient-induced birefringence of CO₂ and CS₂". *Chem. Phys. Lett.* **326** (2000) 269-276
19. S. Coriani, P. Jørgensen, O. Christiansen and J. Gauss. "Triple excitation effects in coupled cluster calculations of Verdet constants". *Chem. Phys. Lett.* **330** (2000) 463-470
20. S. Coriani, A. Halkier, A. Rizzo. "The electric-field-gradient-induced birefringence and the determination of molecular quadrupole moments". Recent Res. Devel. Chem. Physics, Ed. G. Pandalai, Transworld Scientific, Trivandrum, Kerala, India, Vol. **2**, pp. 1-21, 2001.
21. D. Jonsson, P. Norman, H. Ågren, A. Rizzo, S. Coriani, K. Ruud. "The Cotton-Mouton effect of gaseous CO₂, N₂O, OCS and CS₂. A Cubic Response MCSCF study". *J. Chem. Phys.* **114** (2001) 8372-8381
22. A. Halkier and S. Coriani. "State-of-the-art ab initio calculations of the molecular electric quadrupole

- moments of hydrogen fluoride". *Chem. Phys. Lett.* **346** (2001) 329-333
23. A. Rizzo, S. Coriani, B. Fernandez, O. Christiansen. "A coupled cluster response study of the electric dipole polarizability and first and second hyperpolarizabilities of HCl". *Phys. Chem. Chem. Phys.* **4** (2002) 2884-2890
 24. M. Pecul, S. Coriani. "The effect of triple excitations in coupled cluster calculations of Raman scattering cross sections". *Chem. Phys. Lett.* **355** (2002) 327-338
 25. S. Coriani, M. Pecul, A. Rizzo, P. Jørgensen, M. Jaszunski. "Ab initio study of magnetochiral birefringence". *J. Chem. Phys.* **117** (2002) 6417-6428
 26. K. Hald, A. Halkier, P. Jørgensen, S. Coriani. "Orbital nonrelaxed coupled cluster singles and doubles with perturbative triples corrections calculations of first-order one-electron properties". *J. Chem. Phys.* **117** (2002) 9983-9990
 27. K. Hald, A. Halkier, P. Jørgensen, S. Coriani, C. Hättig, T. Helgaker. "A Lagrangian, integral-density direct formulation and implementation of the analytic CCSD and CCSD(T) gradients". *J. Chem. Phys.* **118** (2003) 2985-2998.
 28. S. Coriani, A. Halkier, D. Jonsson, J. Gauss, A. Rizzo, O. Christiansen. "On the electric-field-gradient induced birefringence and the molecular electric quadrupole moments of CO, N₂O and OCS". *J. Chem. Phys.* **118** (2003) 7329
 29. D. Marchesan, S. Coriani, A. Rizzo. "Density dependence of the electric-field-gradient induced birefringence of the helium, neon and argon gases". *Mol. Phys.* **101** (2003) 1851
 30. C. Cappelli, U. Ekström, A. Rizzo, S. Coriani. "The molecular electric quadrupole moment and electric-field-gradient induced birefringence (Buckingham effect) of Cl₂", in *Computational Aspects of Electric Polarizability Calculations: Atoms, Molecules and Clusters*, Ed. G. Maroulis, IOS Press, Amsterdam, ISBN 1586034952, p. 365-380;
 31. C. Cappelli, U. Ekström, A. Rizzo, S. Coriani. "The molecular electric quadrupole moment and electric-field-gradient induced birefringence (Buckingham effect) of Cl₂", *J. Comp. Meth. in Sciences and Engineering (JCMSE)* **4** (2004) 365-380.
 32. A. Rizzo, S. Coriani. "Jones birefringences in gases. Ab initio correlated results for atoms and linear molecules". *J. Chem. Phys.* **119** (2003) 11064-11079
 33. J.L. Cacheiro, B. Fernandez, D. Marchesan, S. Coriani, C. Hättig, A. Rizzo. "Coupled cluster calculations of the ground state potential and interaction induced electric properties of the mixed dimers of helium, neon and argon". *Mol. Phys.* **102** (2004) 101-110.
 34. W. Klopper, S. Coriani, T. Helgaker, P. Jørgensen. "First-order relativistic corrections to response properties: The hyperpolarizability of the Ne atom". *J. Phys. B: At. Mol. Opt. Phys.* **37** (2004) 3753-3763.
 35. S. Coriani, T. Helgaker, P. Jørgensen, W. Klopper. "A closed-shell coupled-cluster treatment of the Breit–Pauli first-order relativistic energy correction". *J. Chem. Phys.* **121** (2004) 6591-6598.
 36. A. Rizzo, C. Cappelli, B. Jansik, D. Jonsson, P. Salek, S. Coriani and H. Ågren. "Density functional and electron correlated study of five linear birefringences — Kerr, Cotton-Mouton, Buckingham, Jones and magnetoelectric — in gaseous benzene". *J. Chem. Phys.* **121** (2004) 8814-8830; *ibidem* **129** (2008) 039901 (erratum).
 37. D. Marchesan, S. Coriani, C. Forzato, P. Nitti, G. Pitacco, K. Ruud. "Optical rotation calculation of a highly flexible molecule: the case of paraconic acid". *J. Phys. Chem. A*, **109** (2005) 1449-1453
 38. M. Pecul, D. Marchesan, K. Ruud and S. Coriani. "Polarizable continuum model study of solvent effects on electron circular dichroism parameters". *J. Chem. Phys.* **122** (2005) 024106(1-9)
 39. C. Puzzarini, S. Coriani, A. Rizzo, J. Gauss. "Critical analysis of the spin-rotation constants of CF₂ and CCl₂: a theoretical investigation". *Chem. Phys. Lett.* **409** (2005) 118-123
 40. A. Rizzo, C. Cappelli, B. Jansik, D. Jonsson, P. Salek, S. Coriani, D.J. Wilson, T. Helgaker, and H. Ågren "Density-functional theory study of electric and magnetic properties of hexafluorobenzene in the vapor phase". *J. Chem. Phys.* **122** (2005) 234314; *ibidem* **129**, (2008) 039901 (erratum).
 41. A. Rizzo and S. Coriani. "Birefringences: A challenge for both Theory and Experiment", in "Response Theory and Molecular Properties (A Tribute to Jan Linderberg and Poul Jørgensen)", edited by H.J.Å. Jensen, *Advances in Quantum Chemistry*, **50** (2005) 143-184.

42. S. Coriani, D. Marchesan, J. Gauss, C. Hättig, T. Helgaker, P. Jørgensen. "The accuracy of ab initio molecular geometries for systems containing second-row atoms". *J. Chem. Phys.* **123** (2005) 184107(1-12)
43. C. Forzato, G. Furlan, P. Nitti, G. Pitacco, D. Marchesan, S. Coriani, E. Valentin. "A Combined Experimental and Computational Strategy in the Assignment of Absolute Configurations of 4-Methyl-5-oxo-tetrahydrofuran-3-carboxylic Acids and their Esters". *Tetrahedron: Asymmetry*, **16** (2005) 3011-3023
44. L. Ferrighi, D. Marchesan, K. Ruud, L. Frediani, S. Coriani. "Gauge-origin independent magnetizabilities of solvated molecules using the Polarizable Continuum Model (PCM)" *J. Chem. Phys.* **123** (2005) 204104(1-11).
45. A. Rizzo, S. Coriani, D. Marchesan, J.L. Cacheiro, B. Fernandez, C. Hättig. "Density dependence of electric properties of binary mixtures of inert gases". *Mol. Phys.* **104** (2006) 305-318
46. I. Garcia Cuesta, S. Coriani, P. Lazzeretti, A. M. J. Sanchez de Meras. "From Pentalene to Dicyclopenta[b,g]naphthalene Or The Change towards Delocalized Structures". *ChemPhysChem* **7** (2006) 240-244
47. S. Coriani, A. Haaland, T. Helgaker, P. Jørgensen. "The equilibrium structure of ferrocene". *ChemPhysChem* **7** (2006) 245-249
48. A. Rizzo, C. Puzzarini, S. Coriani, J. Gauss. "The nuclear spin-rotation constants of HCY, HSiY, and SiY₂ (Y=F, Cl). An ab initio study". *J. Chem. Phys.* **124** (2006) 064302(1-10)
49. A. Baranowska, A. Rizzo, S. Coriani. "Optically induced circular and axial birefringences in achiral fluids: an ab initio study of the optical Faraday effect". *Mol. Phys.* **104** (2006) 2173-2192
50. O. Christiansen, S. Coriani, J. Gauss, C. Hättig, P. Jørgensen, F. Pawłowski, A. Rizzo. "Accurate Non-Linear Optical properties for small molecules. Methods and results", in "Non-linear Optical Properties of Matter: From Molecules to Condensed Phases", Series: "Challenges and Advances in Computational Chemistry and Physics", Vol. **1**, pp 51-99. Eds. M. G. Papadopoulos, J. Leszczynski and A. Sadlej. Springer, 2006; ISBN: 1-4020-4849-1.
51. S. Coriani, A. Baranowska, L. Ferrighi, C. Forzato, D. Marchesan, P. Nitti, G. Pitacco, A. Rizzo, K. Ruud. "Solvent effects on the conformational distribution and optical rotation of γ -methyl paraconic acids and esters". *Chirality* **18** (2006) 357-369.
52. A. Baranowska, A. Rizzo, B. Jansik and S. Coriani. "Non linear effects in the interaction of time-dependent fields and chiral systems. A computational investigation." *J. Chem. Phys.* **125** (2006) 054107(1-10)
53. B. Jansik, A. Rizzo, L. Frediani, K. Ruud and S. Coriani. "A combined density functional/polarizable continuum model study of magnetochiral birefringence: Can theory and experiment be brought to agreement?" *J. Chem. Phys.* **125** (2006) 234105(1-9).
54. S. Høst, J. Olsen, B. Jansik, P. Jørgensen, S. Reine, T. Helgaker, P. Salek, S. Coriani. "Towards a black-box linear scaling optimization in Hartree-Fock and Kohn-Sham theories", in "Trends and Perspectives in Modern Computational Science", Lecture Series on Computer and Computational Sciences, Vol. **6**, 2006, pp. 177-189. Eds. G. Maroulis and T. Simos. Brill Academic Publishers. ISBN10:90 04 15541 4
55. P. Salek, S. Høst, L. Thøgersen, P. Jørgensen, P. Manninen, J. Olsen, B. Jansik, S. Reine, F. Pawłowski, E. Tellgren, T. Helgaker and S. Coriani. "Linear-scaling implementation of molecular electronic self-consistent field theory". *J. Chem. Phys.* **126** (2007) 114110(1-16).
56. A. D. Buckingham, S. Coriani, A. Rizzo. "Investigation of Electric-Field-Gradient-induced birefringence in H₂ and D₂". *Theor. Chem. Acc.* **117** (2007) 969-977
57. S. Coriani, S. Høst, B. Jansik, L. Thøgersen, J. Olsen, P. Jørgensen, S. Reine, F. Pawłowski, T. Helgaker, P. Salek. "A linear-scaling implementation of molecular response theory in self-consistent field electronic-structure theory". *J. Chem. Phys.* **126** (2007) 154108.
58. T. Kjærgaard, B. Jansik, P. Jørgensen, S. Coriani and J. Michl. "Gauge-origin independent Coupled-Cluster-Singles-and-Doubles calculation of Magnetic Circular Dichroism of Azabenzenes and Phosphabenzene using London orbitals". *J. Phys. Chem. A*, **111** (2007) 11278-11286.
59. H. Solheim, L. Frediani, K. Ruud and S. Coriani. "An IEF-PCM study of solvent effects on the Faraday B

- term of Magnetic Circular Dichroism". *Theor. Chem. Acc.* **119** (2008) 231-244.
60. M. Kula, C. Cappelli, S. Coriani, A. Rizzo. "An ab-initio study of the magneto-optical rotation of diastereoisomers". *ChemPhysChem* **9** (2008) 462-469.
 61. H. Solheim, K. Ruud, S. Coriani and P. Norman. "Complex polarization propagator calculations of magnetic circular dichroism spectra". *J. Chem. Phys.* **128** (2008) 094103(1-7)
 62. T. Kjærgaard, P. Jørgensen, J. Olsen, S. Coriani and T. Helgaker. "Hartree-Fock and Kohn-Sham Density functional response theory using a second-quantization atomic-orbital formalism suitable for linear scaling". *J. Chem. Phys.* **129** (2008) 054106.
 63. H. Solheim, K. Ruud, S. Coriani and P. Norman. "The A and B terms of magnetic circular dichroism revisited". *J. Phys. Chem. A*, **112** (2008) 9615-9618 (Letter)
 64. A. J. Thorvaldsen, K. Ruud, A. Rizzo, S. Coriani. "Analytic calculations of frequency-dependent hypermagnetizabilities and Cotton-Mouton constants using London atomic orbitals". *J. Chem. Phys.* **129** (2008) 164110 (1-14).
 65. A. J. Thorvaldsen, K. Ruud, K. Kristensen, P. Jørgensen, S. Coriani, T. Helgaker. "A density matrix-based quasienergy formulation of Kohn-Sham density functional response theory using perturbation- and time-dependent basis sets". *J. Chem. Phys.* **129** (2008) 214108(1-27)
 66. A. J. Thorvaldsen, L. Ferrighi, K. Ruud, H. Ågren, S. Coriani, P. Jørgensen. "Analytic ab initio calculations of Coherent anti-Stokes Raman Scattering (CARS)". *Phys. Chem. Chem. Phys.* **11** (2009) 2293-2304.
 67. D. Shcherbin, A. J. Thorvaldsen, K. Ruud, S. Coriani, A. Rizzo. "Analytic calculations of the Buckingham birefringence using London atomic orbitals", *Phys. Chem. Chem. Phys.* **11** (2009) 816-825.
 68. T. Kjærgaard, P. Jørgensen, P. Salek, A. J. Thorvaldsen, S. Coriani. "A gauge-origin independent formulation and implementation of Magneto-optical Activity within atomic-orbital-density based Hartree-Fock and Kohn-Sham response theories". *J. Chem. Theory Comput.* **5** (2009) 1997-2020.
 69. A. M. Teale, S. Coriani, and T. U. Helgaker. "The calculation of adiabatic-connection curves from full configuration-interaction densities: Two-electron systems", *J. Chem. Phys.* **130** (2009) 104111(1-22)
 70. S. Coriani, C. Forzato, G. Furlan, P. Nitti, G. Pitacco, M. Ringholm, K. Ruud. "Synthesis, characterization and assignment of the Absolute Configuration of 4,4-dimethyl-5-oxo-tetrahydrofuran-3-carboxylic acid and its esters: a combined experimental and theoretical investigation". *Tetrahedron: Asymmetry* **20** (2009) 1459-1467.
 71. J. Friedrich, S. Coriani, T. Helgaker, M. Dolg. "Implementation of the Incremental Scheme for One-Electron First-Order Properties in Coupled-Cluster Theory". *J. Chem. Phys.* **131** (2009) 154102 (cover page).
 72. A. M. Teale, S. Coriani and T. Helgaker. "Range-dependent Adiabatic Connections." Accepted for publication in the AIP Conference Proceedings of ICCMSE 2009. Rhodos, September 29-October 4, 2009
 73. S. Coriani, T. Kjærgaard, P. Jørgensen, K. Ruud, J. Huh, R. Berger. "An atomic-orbital based Lagrangian approach for calculating geometric gradients of linear response properties", *J. Chem. Theory Comput.* **6** (2010) 1028-1047
 74. A. M. Teale, S. Coriani and T. Helgaker, "Accurate calculation and modeling of the adiabatic connection in density functional theory", *J. Chem. Phys.* **132** (2010) 164115
 75. A. M. Teale, S. Coriani and T. Helgaker, "Range-dependent Adiabatic Connections", *J. Chem. Phys.* **133**, 164112 (2010).
 76. A. Rizzo, S. Coriani and K. Ruud, "Response Function Theory Computational Approaches to Linear and Non-Linear Optical Spectroscopy", in "Computational Strategies for Spectroscopy. From Small Molecules to Nano Systems", Editor Vincenzo Barone, Chapter 2, pp. 77-135, 2012. John Wiley and Sons.
 77. S. Coriani, A. J. Thorvaldsen, K. Kristensen, P. Jørgensen, "Variational response function formulation of Vibrational Circular Dichroism", *Phys. Chem. Chem. Phys.* **13** (2011) 4224-4229 DOI: 10.1039/C0CP02230F, Communication
 78. W. Klopper, A.M. Teale, S. Coriani, T.B. Pedersen, T. Helgaker. "Spin-flipping in ring-coupled-cluster-

- doubles theory". Chem. Phys. Letters **510** (2011) 147-153. DOI:10.1016/j.cplett.2011.04.101
79. T. Kjærgaard, K. Kristensen, J. Kauczor, P. Jørgensen, S. Coriani, A. J. Thorvaldsen. "Comparison of standard and damped response formulations of Magnetic Circular Dichroism", J. Chem. Phys. **135** (2011), 024112.
80. M. Strømsheim, N. Kumar, S. Coriani, E. Sagvolden, A. Teale, and T. Helgaker. "Dispersion interactions in density-functional theory: an adiabatic connection analysis". J. Chem. Phys. **135**, (2011) 194109 (1-16)
81. T. Kjærgaard, S. Coriani, K. Ruud. "Ab initio Calculation of Magnetic Circular Dichroism". Invited Overview. *WIREs Computational Molecular Science* (Wiley) **2** (2012) 443-455
82. T. Helgaker, S. Coriani, K. Kristensen, P. Jørgensen, J. Olsen, K. Ruud. "Recent Advances in Wave Function-based Methods of Molecular Property Calculations". Chem. Rev. **112** (2012) 543-631
83. Sonia Coriani, Ove Christiansen, Thomas Fransson, Patrick Norman. "An asymmetric Lanczos-chain driven implementation of electronic resonance convergent coupled cluster linear response theory", J. Chem. Theory Comp. **8**, (2012) 1616-1628
84. S. Coriani, O. Christiansen, T. Fransson, P. Norman. "Coupled-cluster response theory for near-edge x-ray absorption fine structure of atoms and molecules". Phys. Rev. A **85**, (2012) 022507

B. Computer codes

- *LSDALTON, a linear scaling molecular electronic structure program, Release Dalton2011 (2011)*, see <http://daltonprogram.org/>. Written by S. Coriani, T. Helgaker, S. Høst, B. Jansik, P. Jørgensen, J. Kauczor, T. Kjaergaard, K. Kristensen, J. Olsen, S. Reine, P. Salek, A. Thorvaldsen, L. Thøgersen, V. Rybkin, V. Bakken, M. Watson, and A. Krapp
- *DALTON, a molecular electronic structure program, Release Dalton2011 (2011)*, see <http://daltonprogram.org/> Written by C. Angeli, K. L. Bak, V. Bakken, O. Christiansen, R. Cimiraglia, S. Coriani, P. Dahle, E. K. Dalskov, T. Enevoldsen, B. Fernandez, L. Ferrighi, L. Frediani, C. Hättig, K. Hald, A. Halkier, H. Heiberg, T. Helgaker, H. Hettema, B. Jansik, H. J. Aa. Jensen, D. Jonsson, P. Jørgensen, S. Kirpekar, W. Klopper, S. Knecht, R. Kobayashi, J. Kongsted, H. Koch, A. Ligabue, O. B. Lutnæs, K. V. Mikkelsen, C. B. Nielsen, P. Norman, J. Olsen, A. Osted, M. J. Packer, T. B. Pedersen, Z. Rinkevicius, E. Rudberg, T. A. Ruden, K. Ruud, P. Salek, C. C. M. Samson, A. Sanchez de Meras, T. Saue, S. P. A. Sauer, B. Schimmelpfennig, A. H. Steindal, K. O. Sylvester-Hvid, P. R. Taylor, O. Vahtras, D. J. Wilson, and H. Ågren
- "DALTON, an ab initio electronic structure program, Release 2.0", 2005. See <http://www.kjemi.uio.no/software/dalton/dalton.html> by C. Angeli, K. L. Bak, V. Bakken, O. Christiansen, R. Cimiraglia, S. Coriani, P. Dahle, E. K. Dalskov, T. Enevoldsen, B. Fernandez, C. Hättig, K. Hald, A. Halkier, H. Heiberg, T. Helgaker, H. Hettema, H. J. Aa. Jensen, D. Jonsson, P. Jørgensen, S. Kirpekar, W. Klopper, R. Kobayashi, H. Koch, A. Ligabue, O. B. Lutnæs, K. V. Mikkelsen, P. Norman, J. Olsen, M. J. Packer, T. B. Pedersen, Z. Rinkevicius, E. Rudberg, T. A. Ruden, K. Ruud, P. Salek, A. Sanchez de Meras, T. Saue, S. P. A. Sauer, B. Schimmelpfennig, K. O. Sylvester-Hvid, P. R. Taylor, O. Vahtras, D. J. Wilson, H. Ågren.
- "DALTON, an ab initio electronic structure program, Release 1.2", 2001. T. Helgaker, H. J. Aa. Jensen, P. Jørgensen, J. Olsen, K. Ruud, H. Ågren, A. A. Auer, K. L. Bak, V. Bakken, O. Christiansen, S. Coriani, P. Dahle, E. K. Dalskov, T. Enevoldsen, B. Fernandez, C. Hättig, K. Hald, A. Halkier, H. Heiberg, H. Hettema, D. Jonsson, S. Kirpekar, R. Kobayashi, H. Koch, K. V. Mikkelsen, P. Norman, M. J. Packer, T. B. Pedersen, T. A. Ruden, A. Sanchez, T. Saue, S. P. A. Sauer, B. Schimmelpfennig, K. O. Sylvester-Hvid, P. R. Taylor, O. Vahtras".

C. Other publications

- Sonia Coriani, A.J. Thorvaldsen, D. Shcherbin, K. Ruud, K. Kristensen, P. Jørgensen, A. Rizzo. "Density-

matrix based methods for the open-ended analytic calculation of higher-order molecular properties". Scientific Report. In "Relazione Scientifica Settore Calcolo Intensivo", Università degli Studi di Trieste (2009)

- S. Coriani. "*Molecular properties: atomic-orbital based response theories and magnetic circular dichroism simulations*". Scientific Report. In "Relazione Scientifica Settore Calcolo Intensivo", Università degli Studi di Trieste (2008)
- S. Coriani. "*Molecular Response Properties of large systems: recent developments*". Scientific Report. In "Relazione Scientifica Settore Calcolo Intensivo", Università degli Studi di Trieste (2007)
- S. Coriani, D. Marchesan, A. Rizzo. "*Ab initio determination of molecular properties with chemical accuracy*". Technical Report. In "Science and Supercomputing at CINECA. 2005 Report", (2006); ISBN 88-86037-16-3.
- S. Coriani, D. Marchesan, A. Rizzo. "*Ab initio determination of molecular properties with chemical accuracy*". Scientific Report. In "Relazione Scientifica Settore Calcolo Intensivo", Università degli Studi di Trieste (2006)
- S. Coriani: "*Ab initio determination of molecular properties*". Ph.D. Thesis. Aarhus University, July 2000
- S. Coriani. "*Ab initio determination of linear and non-linear optical, electric and magnetic molecular properties*". Progress report, forskeruddannelsens del A, Kemisk Institut, Aarhus Universitet, June 1998.
- S. Coriani. "*Densità di Corrente Elettronica Indotta da Campi Magnetici e Momenti di Dipolo Nucleare Magnetico in Molecole*". Tesi di Laurea in Chimica (M.Sc. thesis in Chemistry), Università degli Studi di Modena, Luglio 1993 (July 1993).