SONIA CORIANI – COMPLETE CURRICULUM VITÆ ET STUDIORUM

Place and date of birth, citizenship: Sassuolo (MO), Italy, 14-12-1968; Italian
Civil Status: Married, two children (born 2003 and 2006)
E-mail: coriani@units.it
Languages: Italian (mother tongue), fluent in English and Danish, reads French and Norwegian.

Academic career

1999–: Tenured assistant professor (*ricercatore*) in Physical Chemistry, Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, Italy;
2010–2012 Associate professor, Marie Curie IEF fellow (FP7-PEOPLE-2009-IEF), Institut for Kemi, Aarhus University, Denmark (01.04.2010–31.1.2012);
2007–2011 Associate professor II, Centre for Theoretical and Computational Chemistry, Kjemisk Institutt, University of Oslo, Norway (20% position, 01.07.2007–01.01.2012);
1997–2000: PhD student, Marie Curie TMR fellow (ERBFMBICT971922), Kemisk Institut, Aarhus University
1997, Feb–Jun: Research assistant (*forskningsassistent*), Kemisk Institut, Aarhus University, DK
1996 (6 months): Visiting Scholar, DRC fellow, Kemisk Institut, Aarhus University
1995 (11 months): Research trainee, Istituto di Chimica Quantistica ed Energetica Molecolare, Pisa, Italy (grant from the Italian Research Council and the European Commission)

Career breaks:

2006, May–October: Maternity leave
2003, Sept–2004 March: Maternity leave

Other professional experiences

1994-1995: Consultant at the Pharmaceutical Packaging Company "Lamp San Prospero S.p.A.", San Prospero s/S, Italy, responsible for the implementation of a Quality Control Laboratory
1993-1994: Teacher in Chemistry and Merceology at the High School "IPSSCT Elsa Morante", Sassuolo, Italy.

Memberships & Affiliations

–Affiliated to the Consorzio Interuniversitario Nazionale per la Scienza e la Tecnologia dei Materiali (INSTM – Consortium for Material Science and Technology), Italy (see www.instm.it)

Administrative experience

2004-2008: Elected member of the Steering Board, Dipartimento di Scienze Chimiche (DSCH), Università degli Studi di Trieste
2005/2006 Member of the departmental committee responsible for the implementation of the „Progetto Lauree Scientifiche" program at DSCH
2001-2007 Coordinator of an Erasmus/Socrates Exchange Agreement between the Dipartimento di Scienze Chimiche, Università degli Studi di Trieste and the Faculty of Chemistry at the University of Santiago de Compostela, Spain.

Education, research training and key qualifications

2010, February: Norwegian Qualification as Full Professor
***2000, Oct 25*:** *Ph.D. degree in Science*, The Faculty of Science, University of Aarhus, Denmark. Ph.D. thesis on "Ab initio determination of molecular properties". Opponents: Prof. A. D. Buckingham (Cambridge, UK) and Prof. J.F. Stanton (Austin, USA).
***1998, July 19*:** Graduate School Qualifying Exam, Faculty of Science, University of Aarhus. Progress report: "Ab initio determination of linear and non-linear optical, electric and magnetic molecular

properties".
***1997, Jul–2000, Jul.*:** Ph.D. student at the Department of Chemistry, University of Aarhus, Denmark, supervised by Prof. P. Jørgensen. Three-years individual Ph.D. stipend from the Marie Curie Training and Mobility of Researchers Programme (FP4), Contract No. ERBFMBICT971922. Research project on: "Theoretical study of static and frequency-dependent optical and magneto-optical properties".
1996, Jan–Jun; Nov–Dec: Visiting scholar at the Division for Theoretical Chemistry, University of Aarhus with fellowship from The Danish Rectors' Conference. Research project: "Gauge-invariant determination of Magnetic Circular Dichroism within the Response Function formalism", supervisor Prof. Poul Jørgensen
1995, Mar–1996, Feb: Research trainee at the Istituto di Chimica Quantistica ed Energetica Molecolare (ICQEM) in Pisa, Italy. Fellowship from the Italian National Research Council (CNR). Supervisor: Dr. A. Rizzo. Research project on: "Theoretical determination of linear and non-linear molecular response properties to electromagnetic perturbations''.
1994: One-year pre-doctoral training course on "Methodologies of laboratory research", Department of Chemistry, University of Modena. Advisor: Prof. P. Lazzeretti.
1993, July 22: Italian 5-years degree (*Laurea*) in Chemistry *cum laude*, University of Modena, Italy. One-year graduation work in Theoretical and Computational Chemistry on "Electronic Current Density Induced by Magnetic Fields and Nuclear Magnetic Moments in Molecules". Supervisor: Prof. P. Lazzeretti.
1987-1993 Chemistry Student at the University of Modena, Italy.

Short- and long-term scientific visits
Apr 1 2010-Jan 31 2012: IEF fellow (*lektor*) at the Department of Chemistry, Aarhus University, Denmark
Jul-Dec 2009: Guest Ass. Prof. at the Department of Chemistry, Aarhus University, DK (sabbatical leave)
Aug 2008/1 month: Guest Ass. Prof. at the Department of Chemistry, Aarhus University, Denmark
Aug 2007/1 month: Guest Ass. Prof. at the Department of Chemistry, Aarhus University, Denmark
June 2005/2 weeks: Visiting scientist, Department of Chemistry, Aarhus University, Denmark
Sept 2004/2 weeks: Visiting scientist, Department of Chemistry, Santiago de Compostela, Spain (FEDER grant)
Sept 2003/1 week: Visiting scientist, Department of Chemistry, University of Tromsø, Norway
Jun 2003/3 weeks: Visiting scientist, Department of Chemistry, Aarhus University, Denmark (
Apr 2003/1 week: Visiting scientist, Department of Chemistry, Aarhus University, Denmark (COST short-term mobility grant)
Mar 2003/3 weeks: Guest Ass. Prof., Department of Chemistry, Santiago de Compostela, Spain (visiting Grant from the Socrates Staff-Exchange Programme)
Feb 2003/1 week: visiting scientist, IPCF-Pisa, Italy
Oct 2002/3 weeks: visiting scientist, Department of Chemistry, Aarhus University, Denmark
May 2002/2 weeks: visiting scientist, Department of Theoretical Chemistry, Lund University, Sweden (Santander grant, visiting O. Christiansen)
Mar. 2002/2 weeks: visiting scientist, Dep.nt of Theoretical Chemistry, Lund University, Sweden (Santander grant, visiting O. Christiansen)
Oct 2001/2 weeks: visiting scientist, Department of Chemistry, Aarhus University
Oct 2001/1 week: visiting scientist, DCCI, University of Pisa, Italy
Jun. 2001/1 month: visiting scientist, Department of Chemistry, Aarhus University, Denmark
May 2001/1 week: visiting scientist, IPCF-Pisa, Italy
Jan 2001/1 week: visiting scientist, Department of Chemistry, Santiago de Compostela, Spain
Nov 2000/3 weeks: visiting scientist, Department of Chemistry, University of Oslo, Norway
Oct 2000/1 month: Department of Chemistry, Aarhus University, Denmark
Jul 2000/1 week: IPCF-Pisa, Italy
Feb 2000/2 weeks: visiting scientist, Inst. for Nanotechnology, Forschungszentrum Karlsruhe, Germany
Jan 2000/1 week: visiting scientist, Department of Chemistry, Utrecht University, The Netherlands

Jun 1998/2 weeks: visiting scientist, IQCEM, Pisa, Italy

Publications

To date more than 80 original scientific papers on international peer-reviewed journals, including 4 reviews and 3 book chapters. In addition: one Ph.D. thesis, one progress report, one master thesis in chemistry, and five scientific reports.

Current *H-index:* ***22*** (as to March 2012)

Contributor to the DALTON (releases 1.2, 2.0 and 2011) and LSDALTON (release 2011) quantum chemistry programs (http://www.daltonprogram.org).

Present and past participation to major research projects and networks

2011-2013 Vice-coordinator of the Trieste node in a "PRIN2009-Progetti di ricerca di Interesse Nazionale" network. Local project "Theory and computational simulation of linear and non linear absorption and ionization processes". Project coordinator: Prof. P. Decleva.

2011 Co-proposer. Exchange Program Project in EuroMagNET II: "Magnetochiral birefringence and dichroism effects: can theory and experiment be brought to agreement". Receiving institution: Laboratoire National des Champs Magnetique Intenses - LNCMI, Toulouse, France.

2010-2012 Individual Intra-European Fellowship for Career Development (IEF), FP7-PEOPLE-2009-IEF funding scheme (recipient). Research project: "Coupled-cluster methods for theoretical x-ray spectroscopies". Grant Agreement nr. 254326. Grant: 265000 Euro.

2007-2012 Affiliated (as Ass. Prof. II) to the Centre for Theoretical and Computational Chemistry (CTCC), University of Oslo, Norway.

2008-2011 Participant in the research project "Analytic calculations of higher-order molecular properties", financed by the Norwegian Research Council. Project leader Prof. Kenneth Ruud.

2009-2012 Participant in the research project "Molecules in Magnetic Fields", coordinated by Prof. Trygve Helgaker, Norwegian Research Council

2006-2008 Co-investigator, Research Project "Molecular Quantum Mechanics: computational methods and analysis of new phenomena", financed by the Italian Ministero per l'Università e la Ricerca (PRIN2006 funding scheme). Research network of four Italian universities. National coordinator: Prof. F. Gianturco; Local coordinator: Prof. P. Decleva. Amount of funding to the Trieste unit: 33000 Euro.

2004-2007 Senior scientist, EU Marie Curie Research and Training network "NANOQUANT: Understanding Nanomaterials from the Quantum Perspective", contract No. MRTNCT-2003-506842 (ended 31/03/2007). Amount of funding to the Pisa node: 163946 Euro.

2002-2007 Node leader, COST Chemistry Working Group D26/012/02, "Towards a new level of accuracy in computations of molecular structure, molecular properties, spectroscopy and thermochemistry", COST Action D26: Integrative Computational Chemistry. Action's coordinator: Prof. J. Noga.

2004-2006 Co-investigator, research project "Theoretical models and computational algorithms to spectroscopic observables and molecular properties" financed by the Italian Ministero dell'Istruzione, Università e Ricerca (PRIN2004 funding scheme). National coordinator: Prof. F. Gianturco; Local coordinator: Prof. P. Decleva. Amount of funding to the Trieste node: 65700 Euro.

2002-2005 Participant, Research project "Optical and magnetic non-linear properties of interacting systems" granted by Spanish Ministry of Science and Technology and by FEDER, Ref. N. BQU2002-02484, University of Santiago de Compostela, Spain. Coordinator: Prof. Berta Fernandez. Amount of funding: 96600 euros.

2000-2002 Co-investigator, research project "Theoretical Models and Computational Techniques for the determination of structural, dynamic and spectroscopic properties of gas-phase molecules and molecular clusters" financed by the Italian Ministero della Ricerca Scientifica e Tecnologica (COFIN2000 funding scheme). Research network of 7 Italian universities. National coordinator: Prof. F. Gianturco; Local coordinator: Prof. G. De Alti. Total amount of funding to the whole network 570684

euros.
2000-2002 Co-investigator, research project "Studio della struttura elettronica e del continuo elettronico di atomi e molecole" financed by the University of Trieste. Coordinator: Prof. G. De Alti.

National and International Schools attended

2002 Winter School in Theoretical Chemistry 2002 "Large Molecules: Linear Scaling and Related Electronic Structure Calculation Methods", Helsinki, Finland.
2000 Winter School in Theoretical Chemistry 2000 "Magnetic properties of molecules", Helsinki, Finland.
2000 Winter School "Modern Methods and Algorithms of Quantum Chemistry", Jülich, Germany.
1997 European Summer School in Quantum Chemistry, ESQC 97, Tjörnarp, Sweden.
1996 Winter School on "Nuclear Quadrupole moments", Helsinki, Finland.
1996 NATO Advanced Study Institute "Problem Solving in Computational Molecular Science: Molecules in Different Environments", Bad Windsheim, Germany.
1996 The Fourth Summer School of Quantum Chemistry and Molecular Properties. Himmelbjergegnens Natur- og Idraetsefterskole, Denmark.
1995 HCM Summer School on Hartree-Fock Theory of Electronic Structure of Solids. Villa Gualino (TO), Italy.
1995 Quarta scuola estiva di elaborazione vettoriale e parallela del CINECA (The Fourth CINECA Summer School on Programming on Vector and Parallel Machines). Casalecchio di Reno (BO), Italy.
1993 Seminario introduttivo alle tecnologie informatiche in Chimica (Seminar on Computational Techniques in Chemistry). IBM Foundation and University of Perugia, Italy.

Personal contributions at national/international Conferences and Meetings:

1. *Invited talk* at IMAMPC 2012, International Meeting on Atomic and Molecular Physics and Chemistry, Pisa, Italy, September 12-14, **2012**
2. *Invited talk* at "Accurate Methods for Accurate Properties", International Symposium in occasion of Peter R. Taylor's 60th birthday, June 4-6, **2012**, Zurich, Switzerland
3. *Invited talk* at "Electronic Structure Theory for Strongly Correlated Systems", May 30-June 1, **2012**, Palermo, Italy
4. *Oral contribution:* S. Coriani, *Coupled cluster study of x-ray near-edge x-ray absorption spectra*. ISTCP-VII: 7th congress of the International Society of Theoretical Chemical Physics. Waseda University, Tokyo, Japan, September 02-08, **2011**
5. *Oral contribution:* S. Coriani, O. Christiansen, T. Fransson, P. Norman. *Coupled cluster study of x-ray near-edge x-ray absorption spectra*. Ninth Triennal Congress of the World Association of Theoretical and Computational Chemists (WATOC-2011), Santiago de Compostela, Spain, July 17-22, **2011**
6. *Contributed talk:* S. Coriani. *Coupled cluster study of x-ray absorption spectroscopy: Near-edge x-ray fine structure from Lanczos-chain driven damped coupled cluster response theory*, CECAM Workshop: X-ray Spectroscopy : Recent Advances in Modelling and New Challenges, CECAM-ETHZ, Zurich, Switzerland, July 13-15, **2011**
7. *Contributed talk:* S. Coriani. *Coupled cluster study of x-ray absorption spectroscopy: Near-edge x-ray fine structure from Lanczos-chain driven damped coupled cluster response theory*. European Seminar on Computational Methods in Quantum Chemistry 2011 (ESCMQC'11), Oscarsborg Fortress, Drøbak, Norway, June 16-19, **2011**
8. *Invited talk:* S. Coriani. *Coupled cluster study of x-ray absorption spectroscopy: Near-edge x-ray fine structure from Lanczos-chain driven damped coupled cluster response theory.* The Danish Chemical Society Annual Meeting 2011, The University of Southern Denmark, Odense, Denmark, June 9, **2011**
9. *Invited talk:* S. Coriani. *Density-matrix based formulation of KS response theory with applications to linear and non-linear spectroscopies.* Nordic-Chinese symposium on Molecular Bio- and

Nanoscience. Hefei, People's Republic of China, September 20-25, **2010**

10. *Plenary lecture:* S. Coriani*. Geometrical and magnetic gradients of linear response properties: A Lagrangian approach.* XXXV Congress of Theoretical Chemists of Latin Expression (XXXV QUITEL). San Andrés. Colombia, September 18-22, **2009**
11. *Poster*: S. Coriani, T. Kjærgaard, P. Jørgensen, A. Thorvaldsen, K. Ruud, R. Berger. *In silico determination of optical and spectroscopic properties: a few recent methodological and applicative results*. "Molecular Properties - MP'09 - Bridging the gap between theory and experiment. An ICQC 2009 satellite symposium". June 18-21, **2009,** Oslo, Norway
12. *Oral contribution:* S. Coriani. *In silico determination of magnetic circular dichroism parameters and spectra*. Workshop "Nanoscale Modelling of new molecular experiments: Theoretical and Computational Simulations" . Roma, March 6th **2009**
13. *Invited communication*: S. Coriani. *In silico determination of magnetic circular dichroism parameters and spectra*. "Winter Modeling 2008", Pisa, Italy. December 19, **2008**
14. *Invited talk*: S. Coriani. *In silico determination of magnetic circular dichroism parameters and spectra*. "Trends in quantum chemistry. A meeting for the future purposes and methods". Lundbeck Foundation Center for Theoretical Chemistry at Aarhus University, Dec. 12-14, **2008**
15. *Oral communication*: S. Coriani. *Molecular Response Properties of large systems: recent developments*. "XXXVII Congresso Nazionale della Sezione di Chimica Fisica della Società Chimica Italiana". Camogli, Genova, February 28, **2008**
16. *Invited talk*: S. Coriani. *A Linear-Scaling Implementation of Molecular Response Theory in Self-Consistent Field Electronic-Structure Theory*. "NANOQUANT, the end-of-the-project meeting, WARSAW 2007". Hotel Sobieski, Warsaw, March 16-17, **2007**
17. *Poster*: S. Coriani, S. Høst, B. Jansik, L. Thøgersen, J. Olsen, P. Jørgensen, S. Reine, F. Pawlowski, T. Helgaker and P. Salek. *A linear-scaling implementation of molecular response theory in self-consistent electronic structure theory*. "VI Convegno Nazionale del Gruppo Interdivisionale di Chimica Computazionale della Società Chimica Italiana (GICC06)", Isola di San Servolo, Venezia. December 18-21, **2006**.
18. *Invited Talk*: S. Coriani. *On the Buckingham Birefringence in Atoms and Molecules*. "Linear and Non-linear Optical Properties. A Theoretical Chemistry Symposium dedicated to Professor A. D. Buckingham", International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2006), Chania, Crete. October 27-November 1 **2006**
19. *Invited talk*: S. Coriani. *Recent developments in the determination of molecular properties: Atomic orbital based Response Theory*. "XIII European Seminar on Computation Methods in Quantum Chemistry (XIII Strasbourg Seminar)". Smolenice, Slovak Republic. 21-25 September **2005**
20. *Oral communication*: S. Coriani. *Determinazione di proprietà molecolari con metodi di struttura elettronica: il programma Dalton*. "Workshop Introduttivo per il nuovo Centro Interdipartimentale per le Scienze Computazionali (CISC)". Università di Trieste, June 15, **2005**
21. *Oral communication*: S. Coriani. *Report of the Working Group 12: Towards a new level of accuracy in computations of molecular structure, molecular properties, spectroscopy and thermo-chemistry. Part II*. "COST Chemistry D26, Integrative Computational Chemistry. Midterm Evaluation Conference". Fisher's Hotel, Pitlochry, Scotland. 5-8 May **2005**
22. *Oral communication*: S. Coriani. *On the accurate determination of molecular structures and frequency dependent properties*. "Mid-term evaluation Meeting of the COST Chemistry Action D26/012/02". Karlsruhe, Germany, January 26, **2005**
23. *Invited talk*: S. Coriani, D. Marchesan, C. Hättig, T. Helgaker, P. Jørgensen. *On the accurate determination of static and frequency dependent molecular properties*. "Italian-Norwegian-Swedish Workshop on Quantum Molecular Sciences", Tromsø, Norway. September, 17-20 **2004**
24. *Poster:* S. Coriani, D. Marchesan, C. Hättig, T. Helgaker, P. Jørgensen. *Accurate geometries from ab initio calculation: systems containing second row atoms*. "Molecular Quantum Mechanics: the No Nonsense Path to Progress. An International Conference in Honour of Professor Nicholas Handy". Cambridge (UK) July 24-29, **2004**
25. *Poster*: D. Marchesan, S. Coriani, C. Forzato, P. Nitti, G. Pitacco, K. Ruud. *The solvent effect on*

conformational distributions and optical activity of paraconic acid family of gamma-butyrolactones. "Divisione di Chimica Fisica – Società Chimica Italiana, XXXIII Congresso Nazionale". Napoli - Complesso Universitario di Monte S. Angelo, June 21-25, **2004**.

26. Poster: A. Rizzo, S. Coriani, M. Pecul, M. Jaszunski, P. Jørgensen. *Birefringences: Recent Developments*. "Twelfth European Seminar on Computational Methods in Quantum Chemistry (XII Strasbourg Seminar)", Zeist, The Netherlands, September 18-22, **2002**.
27. Poster: S. Coriani, K. Hald, A. Halkier, C. Hättig, P. Jørgensen, T. Helgaker. *A Lagrangian, integral-density direct formulation of the analytic CCSD and CCSD(T) gradients*. "Twelfth European Seminar on ComputationalMethods in Quantum Chemistry (XII Strasbourg Seminar)", Zeist, The Netherlands, September 18-22, **2002**.
28. Invited communication: S. Coriani, A. Rizzo, M. Pecul, M. Jaszunski, P. Jørgensen. *Ab initio investigation of magnetochiral birefringence*. "Midterm Review Meeting and Second Network Coordination Meeting for the European HPRN network Molecular Properties and Molecular Materials HPRN-2000-00013 (MOLPROP)", Gentofte, Denmark, January 24–26, **2002**
29. Oral communication: S. Coriani. *Molecular properties within coupled cluster response theory*. "Riunione Scientifica del Programma di Ricerche Cofinanziate MURST 2000-2002 (ex 40%)", Roma, Italy, June 27-28, **2001**
30. Oral communication: S. Coriani. *The electric field gradient induced birefringence and the molecular quadrupole moments of linear molecules*. "EU/RTN network meeting on: Molecular properties and molecular materials (MOLPROP)", Stockholm, Sweden, May 28-29, **2000**.
31. Oral communication: S. Coriani. *Linear birefringence effects and magneto-optical activity within coupled cluster response theory: the electric-field-gradient induced birefringence of atoms and molecules*. "30-aars jubilaeumssymposium. Sektionen for Teoretisk Kemi, Kemisk Forening", Odense, Denmark, October 19, **1999**.
32. Poster: S. Coriani. *Gauge-origin independent magneto-optical activity within coupled cluster response theory*. "7th International Conference on Circular Dichroism", Mierki, Poland, August 25–29, **1999**
33. Poster: A. Rizzo, S. Coriani, C. Hättig, A. Halkier. *The electric-field-gradient-induced birefringence of a polar molecule: CO*. "American Conference in Theoretical Chemistry, ACTC 99". Boulder, Colorado, USA, June 28–July 2, **1999**
34. Poster: S. Coriani, C. Hättig, P. Jørgensen, T. Helgaker. *Gauge-origin independent magneto-optical activity within coupled cluster response theory*. "American Conference in Theoretical Chemistry, ACTC 99", Boulder, Colorado, USA June 28–July 2, **1999**
35. Oral communication: S. Coriani. *Gauge-origin invariant magneto-optical activity within coupled cluster response theory*. "Italian-Swedish Workshop in Quantum Chemistry", Stockholm, Sweden, June 22–24, **1999**
36. Poster: A. Halkier, H. Larsen, S. Coriani, J. Olsen, P. Jørgensen, J. Gauss. *Electric moments with spectroscopic accuracy from high-level ab initio calculations*. International Conference on "Electron Correlation Effects in Spectroscopy and Dynamics", Kaiserslautern, Germany, December 9–12, **1998**.
37. Poster: S. Coriani, C. Hättig, A. Halkier, P. Jørgensen, A. Rizzo, K. Ruud. *Birefringence effects and magnetooptical activity within Response theory*. International Conference on "Electron Correlation Effects in Spectroscopy and Dynamics", Kaiserslautern, Germany, December 9–12, **1998**
38. Invited communication: S. Coriani. *Magneto-optical properties within response theory*. CECAM workshop "Electronic Response Functions in Atoms, Molecules and Solids" CECAM, ENS, Lyon, France, October 5–7 **1998**
39. Poster: S. Coriani, A. Rizzo, C. Hättig, P. Jørgensen. *The Electric Field Gradient Induced Birefringence Effect in Atoms and Molecules*. Poster. Workshop "From Small to Large IV. High performance computing of non-linear and photonic materials", Linköping, Sweden, March 4–7 **1998**
40. Poster: S. Coriani, A. Rizzo, K. Ruud. T. Helgaker. *Hypermagnetizabilities and nuclear shielding polarizabilities of ethylene: an MCSCF study*. COST workshop "Quantum Systems in Chemistry and Physics", San Miniato (PI), Italy, April **1996**

41. *Oral communication:* S. Coriani, A. Rizzo. *Studio degli effetti di campo elettrico sulle proprietà magnetiche: polarizzabilità di shielding e costante di Cotton-Mouton del CO*. National workshop: "Verso la complessità molecolare, modelli per la dinamica ed i processi reattivi", Monselice (PD), Italy, June 14-17, **1995**.

Invited seminars (from 2007)

1. S. Coriani. "Reliable modeling of light-matter interactions: challenging spectroscopies and exotic molecular properties". Department of Chemistry, University of Helsinki, Helsinki, Finland, April 13, 2012
2. S. Coriani. "In silico determination of spectroscopic properties: a few recent methodological and applicative results". Theoretical Chemistry Colloquia, Ruhr-Universitet Bochum, Germany, July 8, 2009
3. S. Coriani. "Response Function Theory computational approaches to linear and non-linear optical properties and spectroscopies". Dipartimento di Scienze Chimiche, Università degli Studi di Padova, Italy, March 19, 2009
4. S. Coriani. "Challenging the limits of the quantum-chemical modeling of molecular response properties", Lille Auditorium (B203), Realfag, University of Tromsø, Norway, March 11, 2008.
5. S. Coriani. "Molecular Response Properties of large systems: recent developments". Department of Chemistry, Oslo University (Norway), October 19, 2007
6. S. Coriani. "AO-based linear-scaling implementation of molecular response theory in SCF electronic-structure theory". Dip. di Chimica, Università Federico II, Complesso Universitario Monte Sant'Angelo, Napoli. April 17, 2007

Conferences organized

2010: International Workshop "Quantum Chemistry beyond the Arctic Circle – Promoting Female Excellence in Theoretical and Computational Chemistry", Sommarøy and Tromsø, Norway, June 23-26, 2010, http://www.ctcc.no/polar2010 – Main organizer together with Dr. Magdalena Pecul

2008: "XIV European Seminar on Computational Methods in Quantum Chemistry (ESCMQC)", Elba, Italy, October 2-6, 2008, http://h2.ipcf.cnr.it/rizzo/AR_ESCMQC.html – Member of the organizing committee

Peer review activities

1. Referee assignments in international periodicals

Regular referee for: *The Journal of Chemical Physics, Chemical Physics Letters, The Journal of Molecular Structure, European Journal of Physics D, Journal of Computational Methods in Sciences and Engineering, International Journal of Quantum Chemistry, The Journal of Physical Chemistry, Theoretical Chemistry Account, Chemical Physics, Molecular Physics, Journal of Chemical Theory & Computation, Oxford University Press*.

2. Assignments as outside expert

- Proposal evaluator, Italian Ministry of Research (PRIN initiative)
- Pre-proposal evaluation, ERA Chemistry initiative
- Proposal evaluator, FRS-FNR (Belgian research council)
- Proposal evaluator, South-African National Research Foundation (NRF)
- Proposal evaluator, University of Ghent (Belgium)
- Proposal evaluator, Academy of Science for the Developing World (TWAS).
- Member of the expert panel for the assessment of an application for promotion to full professor at the Department of Theoretical Chemistry and Biology, KTH School of Biotechnology (August 2011)

3. Assignments as public examiner/opponent

- Opponent of Ph.D. dissertation of Suvi Ikäläinen, Department of Chemistry, University of Helsinki, Finland, April 13, 2012

- Co-opponent of Ph.D. dissertation of Alberto Zoccante, Department of Chemistry, Aarhus University, Denmark, June 22, 2012
- Evaluation Committee Member of Ph.D. dissertation of Dr. Margret Gruber-Stadler's, Kjemisk Institutt, Oslo University, Norway, November 21, 2008
- Member of the evaluation committee for 2 permanent researcher positions, one at the University of Bologna (2004) and one at the University of Napoli (2008), and for various researcher and post-doctoral positions at the CTCC (in 2007, 2009, 2011, 2012).

IT competences

Code development in Fortran, Python, Shell Scripting.
Operating systems Unix, Linux, Windows, Mac OS X.
Software: Dalton, Gaussian, Molcas, NWChem, Cfour.
Expert user of Latex
Expert user of Office products (Word, Excel, PowerPoint)

TEACHING RECORD

Academic Years 2010-2011 and 2011-2012
– On leave from teaching duties due to IEF grant at Aarhus University
Academic Years 2006-2007, 2007-2008 and 2008-2009
– Lecturer & examiner of compulsory course "Informatics for Chemists" (3 credits or ETC) for the Bachelor degree in Chemistry, University of Trieste. First semester. Code SM461
– Lecturer & examiner of elective course "Molecular Modeling and Simulation: An Introduction" (4 credits or 4ETC) for the Bachelor degree in Chemistry, University of Trieste. Second semester. Code SM266
– Lecturer & examiner of elective course "Programming Techniques in Computational Chemistry" (4 credits or ETC) for the Master degree in Chemistry, University of Trieste. Second semester. Code SM707
Academic Year 2005-2006 (on maternity leave from May to Oct. 2006)
– Lecturer & examiner of compulsory course "Informatics" (3 credits or ETC) for the Bachelor degree in Chemistry, University of Trieste. First semester. Code SM092
– Lecturer & examiner of elective course "Molecular Modeling and Simulation: An Introduction" (4 credits or ETC) for the Bachelor degree in Chemistry, University of Trieste. Second semester. Code SM266
Academic Year 2004-2005
– Lecturer of a PhD course on "Molecular Properties", PhD School in Chemistry, University of Trieste
Academic Year 2003-2004 (on maternity leave from Sept. 2003 to Mar. 2004)
– Lecturer & examiner of elective course "Molecular Modeling and Simulation: An Introduction" (4 credits of ETC) for the Bachelor degree in Chemistry, University of Trieste.
– Responsible for Integrative lectures, preparatory work and assistance during the laboratory experimental activities of the compulsory course "Integrative Laboratory Course. Physical Chemistry part" for the Degree in Environmental Sciences, University of Trieste.
Academic Year 2002-2003
– Lecturer & examiner of a one-week seminar course on "Complements of Quantum Mechanics", Master degree in Chemistry, University of Santiago de Compostela, Spain, within the Socrates Exchange Staff Program
– Lecturer of PhD Course on "Complements of Quantum Mechanics", PhD School in Chemistry, University of Trieste.
– Laboratory Assistant of the compulsory course "General Chemistry Laboratory" (8 credits or ETC) for the Degree in Biological Sciences, University of Trieste.
– Responsible for Integrative lectures, preparatory work and assistance during the laboratory

experimental activities of the compulsory course "Integrative Laboratory Course - Physical Chemistry part" for the Degree in Environmental Sciences, University of Trieste.

Academic Year 2001-2002

– Lecturer & examiner of elective course "Quantum Chemistry" (6 credits), Degree in Chemistry (prior to reformation), University of Trieste

– Responsible for Integrative lectures, preparatory work and assistance during the laboratory experimental activities of the compulsory course "Integrative Laboratory Course - Physical Chemistry part", Degree in Environmental Sciences, University of Trieste.

– Laboratory Assistant of the compulsory course "General Chemistry Laboratory" (6 credits or ETC) for the Degree in Biological Sciences, University of Trieste.

Academic Year 2000-2001

– Responsible for Integrative theoretical lectures, preparatory work and assistance during the laboratory experimental activities of the compulsory course "Integrative Laboratory Course - Physical Chemistry part", for the Degree in Environmental Sciences, University of Trieste.

– Laboratory Assistant of the compulsory course "General Chemistry Laboratory" (6 credits or ETC) for the Degree in Biological Sciences, University of Trieste.

Academic Year 1999-2000

– Instructor, Teoretiske Øvelser i *Kemi 21–Fysisk Kemi* (Numerical Exercises in Chemistry 21-Physical Chemistry), Bachelor Degree in Chemistry, Aarhus University, Denmark.

Academic Year 1998-1999

– Instructor, Teoretiske Øvelser i *Kemi 22–Molekylspektroscopi og Kemisk Binding* (Numerical Exercises in Chemistry 22-Molecular Spectroscopy and Chemical Bonding), Bachelor Degree in Chemistry, Aarhus University, Denmark.

– Instructor, Teoretiske Øvelser i *Kemi 21–Fysisk Kemi* (Numerical Exercises in Chemistry 21-Physical Chemistry), Bachelor Degree in Chemistry, Aarhus University, Denmark.

School Year 1993-1994 (November to June)

– High-school teacher in „Chemistry and Merceology" at the Istituto Professionale di Stato per i Servizi Commerciali e Turistici "Elsa Morante", Sassuolo (MO), Italy.

Student supervision

2002-2004 Supervisor of **PhD student** Dr. Domenico Marchesan, who obtained his Ph.D. degree on April 5, 2005 at the Dipartimento di Scienze Chimiche, University of Trieste.

2004-2005 Co-supervisor of **Ph.D. student** Angelika Baranowska from the University of Torun, during her one-year long research-training period as pre-doctoral trainee within the NANOQUANT project at the Pisa node (6 months entirely spent in my lab). Co-supervised with Dr. A. Rizzo.

2008 Supervisor of **Bachelor student** Mauro Pianca for his Bachelor degree in Chemistry (conferred in July 2008), University of Trieste.

2011 Co-advisor of **Master student** Thomas Fransson from Linkopings universitet, Institute of Tehnology, Department of Physics, Chemistry and Biology during his 10-week long training period at the University of Aarhus. Co-supervised with Prof. O. Christiansen. Examiner Patrick Norman.

Popularisation of Science

From 2004: Proponent and main responsible for the popularization-of-science project: "ChemShow - Chemistry wonders" at the University of Trieste. To date the activity has been attended by more than 1000 pupils (http://www2.units.it/~cird/progetti/chemshow/chemshow.htm).

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 CH_4 ". *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 ^{17}O in $^{16}O^{17}O^{16}O$ and $^{17}O^{16}O^{16}O$". *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 H_2 , N_2 , C_2H_2 and CH_4 ". *J. Chem. Phys.* **109** (1998) 7176-7184
10. A. Halkier, S. Coriani, and P. Jørgensen. "The molecular electric quadrupole moment of N_2". *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 C_2H_2". *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 SF_6 ". *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 CO_2 and CS_2 ". *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

CO_2, N_2O, OCS and CS_2. 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, N_2O 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 Cl_2", 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 Cl_2", *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.
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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 CF_2 and CCl_2 : 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]naphtalene Or The Change towards Delocalized Structures". ChemPhysChem **7** (2006) 240-244
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48. A. Rizzo, C. Puzzarini, S. Coriani, J. Gauss. "The nuclear spin-rotation constants of HCY, HSiY, and SiY_2 (Y=F, Cl). An ab initio study". J. Chem. Phys. **124** (2006) 064302(1-10)
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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. Jansık, S. Reine, F. Pawlowski, 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 H_2 and D_2 ". *Theor. Chem. Acc.* **117** (2007) 969-977
57. S. Coriani, S. Høst, B. Jansik, L. Thøgersen, J. Olsen, P. Jørgensen, S. Reine, F. Pawlowski, 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.
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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)
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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)
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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.
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80. 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, John Wiley & Sons, 2012 (book chapter).
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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. H¨attig, 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

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