

Luca Frediani

Curriculum vitæ

01.06.1975: Born in Livorno, Italy.

July 1993: Bachelor degree at the “Istituto Tecnico Industriale G. Galilei”, Livorno. Grade: 60/60

Academic years from 1993/1994 to 1999/2000: Chemistry studies at the Università degli Studi di Pisa with a Physical Chemistry specialization.

13th October 2000: University degree *summa cum laude* in Chemistry.

Academic years from 1993/1994 to 1998/1999: Chemistry studies at the “Scuola Normale Superiore”, Pisa.

17th October 2000: Diploma of the “Scuola Normale Superiore”. Grade: 70/70 *cum laude*.

January 2001 - December 2003: Ph.D. course in Chemistry under the supervision of Prof. Roberto Cammi. Final defense held on March 18, 2004.

October 2001 and June 2002: Visiting scholar to Prof. Kenneth Ruud, Tromsø, Norway.

January-April 2003: Visiting scholar to Prof. J. T. Hynes’s laboratory in Boulder (Colorado, USA).

April 2003: Visiting scholar at Pacific Northwest National Laboratory, Richland (Washington, USA) to Prof. Bruce Garret’s group.

April 2004-April 2005: Post-Doc in the group of Prof. Hans Ågren at the Royal Institute of Technology, Stockholm, Sweden.

April 2005-April 2007 Post-Doc in the group of Prof. Kenneth Ruud at the Department of Chemistry of the University of Tromsø, Norway.

Since April 2007 Associate Professor in Theoretical Chemistry at the Department of Chemistry, University of Tromsø.

Since July 2007 Senior staff member of the Center for Theoretical and Computational Chemistry.

Schools, congresses and meetings

August 2001: “European Summer school in Quantum Chemistry” Tjörnarp, Sweden. Poster presentation.

July 2002: “7th Sostrup Summer School QUANTUM CHEMISTRY and MOLECULAR PROPERTIES” held in Sostrup, Denmark. Poster presentation.

July 2002: “CCP5 Methods in Molecular Simulation Summer School 2002”, King’s College, London, England.

October 2002: “Yangtze Conference on Fluids and Interfaces”, Nanjing/Chongqing, China. Poster presentation.

November 2002: COST 26 action Meeting in Namur, Belgium.

July 2003: “Multidimensional Reaction Dynamics”, Germany.

July 2003: “XI International Congress in Quantum Chemistry”, Bonn, Germany. Poster presentation.

September 2003: Euresco Conference on molecular liquids entitled: “Routes from Local Order to Large-Scale Cooperativity”, Castelvechio Pascoli, Italy.

September 2003: Conference entitled “A Coastal Voyage in Quantum Chemistry”, Tromsø/Trondheim, Norway.

June 2004: Symposium entitled “*Biophotonics 2004*”, Stockholm, Sweden.

August 2004 “*μ-Theochem: Modelling and Understanding in Theoretical Chemistry*”, Lucca, Italy. Oral presentation.

September 2004: Conference entitled “*Italian-Norwegian-Swedish Workshop on Quantum Molecular Sciences*”, Tromsø, Norway. Oral presentation.

April 2005: COST 26 action meeting Pisa

October 2005: “International Conference of Computational Methods in Sciences and Engineering”, Loutraki, Greece. Oral presentation.

Feb 2006: Mid-term meeting of the European Union Financed Research Network “NanoQuant”. Oral presentation.

May 2006: Conference “Svensk teoretisk kemi” and COST 26 action meeting, Stockholm, Sweden. Oral presentation.

May 2006: Satellite meeting “Chemical Accuracy and beyond”, Tokyo, Japan.

May 2006: “XII International Congress in Quantum Chemistry”, Kyoto, Japan. Poster presentation.

February 2007 “eVITA” research meeting in Geilo, Norway.

May 2007 Conference “Analytical gradients and beyond”, Budapest, Hungary. Poster presentation.

Sept 2007 Swedish Theoretical Chemistry Symposium, Örebro, Sweden. Invited talk.

Dec 2007 Workshop “Nonlinear and Adaptive Approximation in High Dimensions” Physikzentrum Bad Honnef, Germany. Oral presentation.

Jul 2008 Workshop “Numerical methods in Density Functional Theory” Berlin, Germany. Invited talk.

Sept 2008 “XIV European Seminar on Computational Methods in Quantum Chemistry”, Elba, Italy. Invited talk.

Sept 2009 Conference “DFT09”, Lyon, France, Poster presentation.

Languages

Italian (mother tongue), English (fluent), Norwegian (very good), Swedish (intermediate).

IT and computational knowledge

Operating Systems: Linux and Unix

Programming languages: Fortran, C, Perl, C++, Python.

Quantum chemistry software: DALTON, GAUSSIAN and GAMESS

Present and past students supervised

- Arnfinn Hykkerud Steindal (PhD student)
- Dmitry Shcherbin (PhD student, co-supervisor)
- Stig Rune Jensen (Master student, co-supervisor, graduated Dec 2009)
- Stig Rune Jensen (PhD student, supervisor)

Teaching activity

I am teaching the following courses:

- General Chemistry (KJE-1001, bachelor)
- Theoretical Chemistry and Spectroscopy (KJE-2001, bachelor)
- Quantum Chemistry (KJE-3101, master)
- Computational Chemistry (KJE-3102, master)

- Theoretical Chemistry Methods(KJE-3103, master)
- Wavelet Methods in Chemistry and Physics (MAT-8204, PhD)

For all courses except for General Chemistry, I am the main responsible/coordinator.

Grants

- Year 2002, Young researcher grant from the University of Parma (4.000 euro)
- Year 2007, Start-up grant for the establishment of the Wavelet method course (40.000 NOK)
- Year 2008, Research Grant from the Mohn foundation (4.500.000 NOK)
- Year 2009, Young researcher prize from the University of Troms (50.000 NOK)

Fields of interests and research activity

My field of interest is mainly concerned with method development in quantum chemistry.

I have started my research activity by developing a model include the effect of solvation from surfaces and interfaces on a molecular system described quantum mechanically. The method is an extension of the continuum solvation model known as PCM (Polarizable Continuum Model) to treat system with planar surfaces. This is a research activity which I am pursuing also at present by extending the model to more sophisticated environments (e.g. beyond planar surfaces), modelling other solvation energy contributions beyond electrostatics, reformulating the electrostatic problem within the wavelet formalism.

Another branch of my research activity, which is closely related to the previous one, involves the implementation of the PCM in the Dalton Quantum Chemistry Program to model solvent effects on linear and nonlinear molecular properties. This activity has involved mainly the implementation of the solvent contribution to the response equations for Hartree-Fock, Density Functional Theory and Multiconfiguration Self-Consistent Field Theory. The connection of this two activities will allow the modelling of molecular properties for chromophores at surfaces and interfaces.

I am also interested in the development of the integration the of continuum solvation model with the Quantum Mechanics/Molecular Mechanics method. In this way one could model chromophores in condensed phase in a much more realistic, layered way: (1) the chromophores is treated accurately with quantum chemistry methods; (2) the nearby surrounding whose specific interactions with the chromophore are important, is modelled with MM fragments and the bulk solvent, where only mediated long-range interactions are needed is treated through the PCM. In this project is involved the PhD student I am supervising (A. H. Steindal).

In the last years, my research activity has also been concerned with the development and implementation of a code to treat Quantum Chemistry problems with the tools of Multiresolution Analysis. This work has led to the implementation of a Multiwavelet code to apply an operator in the “so-called” Non-Standard form up to any finite arbitrary precision in a space with arbitrary number of dimensions. In particular, we have implemented a Poisson and Helmholtz solver in three dimension which is the basic tool to solve the Kohn-Sham equations of DFT in a Multiwavelet framework.

Publications

- [1] Ville Weijo, Maharavo Randrianarivony, Helmut Harbrecht, and Luca Frediani. Wavelet formulation of the polarizable continuum model. *J Comp. Chem.*, 2010. Published on line.
- [2] Lara Ferrighi, Luca Frediani, and Kenneth Ruud. Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model. *The Journal of Chemical Physics*, 132(2):024107, 2010.
- [3] H. Solheim, L. Frediani, K. Ruud, and S. Coriani. An IEF-PCM study of solvent effects on the Faraday B term of mcd. *Theoretical Chem. Accounts*, 119(1-3):231–244, 2008.
- [4] Harald Solheim, Luca Frediani, Sonia Coriani, and Kenneth Ruud. An IEF-PCM study of solvent effects on the faraday B term of MCD. *Theor. Chem. Acc.*, 2007.
- [5] L. Ferrighi, L. Frediani, E. Fossgaard, and K. Ruud. Two-photon absorption of [2.2]paracyclophane derivatives in solution: A theoretical investigation. *J. Chem. Phys.*, 127(24):244103, 2007.
- [6] L. Ferrighi, L. Frediani, and K. Ruud. Degenerate four-wave mixing in solution by cubic response theory and the polarizable continuum model. *J. Phys. Chem. B*, 111(30):8965–8973, 2007.
- [7] Stefano Corni and Luca Frediani. *Molecules at surfaces and interfaces*, chapter 2.11. Wiley, 2007.
- [8] A. Rizzo, L. Frediani, and K. Ruud. An ab initio investigation of the Buckingham birefringence of furan, thiophene, and selenophene in cyclohexane solution. *J. Chem. Phys.*, 127(16):164321, 2007.
- [9] Ke Zhao, Lara Ferrighi, Luca Frediani, Chuan-Kui Wang, and Yi Luo. Solvent effects on two-photon absorption of dialkylamino substituted distyrylbenzene chromophore. *J. Chem. Phys.*, 126(20):204509, 2007.
- [10] B. Jansik, A. Rizzo, L. Frediani, K. Ruud, and S. Coriani. Combined Density Functional/Polarizable Continuum Model study of magnetochiral birefringence: Can theory and experiment be brought to agreement? *J. Chem. Phys.*, 125(23):234105, 2006.
- [11] M. Pecul, E. Larnparska, C. Cappelli, L. Frediani, and K. Ruud. Solvent effects on Raman optical activity spectra calculated using the Polarizable Continuum Model. *J. Phys. Chem. A*, 110:2807–2815, 2006.
- [12] L. Ferrighi, L. Frediani, C. Cappelli, P. Salek, H. Agren, T. Helgaker, and K. Ruud. Density-functional-theory study of the Electric-Field-Induced Second Harmonic Generation (EFISHG) of push-pull phenylpolyenes in solution. *Chem. Phys. Lett.*, 425(4-6):267–272, 2006.
- [13] L. Ferrighi, L. Frediani, E. Fossgaard, and K. Ruud. Parallelization of the Integral Equation Formulation of the Polarizable Continuum Model for higher-order response functions. *J. Chem. Phys.*, 125(15):154112, 2006.
- [14] L. Bondesson, L. Frediani, H. Agren, and B. Mennucci. Solvation of N_3^- at the water surface: The Polarizable Continuum Model approach. *J. Phys. Chem. B*, 110(23):11361–11368, 2006.
- [15] L. Ferrighi, D. Marchesan, K. Ruud, L. Frediani, and S. Coriani. Gauge-Origin-Independent magnetizabilities of solvated molecules using the Polarizable Continuum Model. *J. Chem. Phys.*, 123:204104, 2005.
- [16] L. Frediani, H. Agren, L. Ferrighi, and K. Ruud. Second-Harmonic Generation of solvated molecules using Multiconfigurational Self-Consistent-Field Quadratic Response Theory and the Polarizable Continuum Model. *J. Chem. Phys.*, 123:144117, 2005.
- [17] L. Frediani, Z. Rinkevicius, and H. Agren. Two-Photon Absorption in solution by means of Time-dependent Density-Functional Theory and the Polarizable Continuum Model. *J. Chem. Phys.*, 122:244104, 2005.

- [18] L. Frediani, R. Cammi, S. Corni, and J. Tomasi. A Polarizable Continuum Model for molecules at diffuse interfaces. *J. Chem. Phys.*, 120:3893–3907, 2004.
- [19] L. Frediani, R. Cammi, C. S. Pomelli, J. Tomasi, and K. Ruud. New developments in the symmetry-adapted algorithm of the Polarizable Continuum Model. *J. Computational Chem.*, 25:375–385, 2004.
- [20] L. Frediani, B. Mennucci, and R. Cammi. Quantum-mechanical continuum solvation study of the polarizability of halides at the water/air interface. *J. Phys. Chem. B*, 108:13796–13806, 2004.
- [21] R. Cammi, B. Mennucci, C. Pomelli, C. Cappelli, S. Corni, L. Frediani, G. W. Trucks, and M. J. Frisch. Second-order Moller-Plesset second derivatives for the Polarizable Continuum Model: theoretical bases and application to solvent effects in electrophilic bromination of ethylene. *Theoretical Chem. Accounts*, 111:66–77, 2004.
- [22] Kenneth Ruud, Benedetta Mennucci, Roberto Cammi, and Luca Frediani. The calculation of excited-state polarizabilities of solvated molecules. *J. Comp. Meth. Sci. Eng.*, 4(3):381–397, 2004.
- [23] K. Ruud, L. Frediani, R. Cammi, and B. Mennucci. Solvent effects on the indirect spin-spin coupling constants of benzene: The DFT-PCM approach. *Int. J. Mol. Sciences*, 4:119–134, 2003.
- [24] R. Cammi, L. Frediani, B. Mennucci, and K. Ruud. Multiconfigurational Self-Consistent Field Linear Response for the Polarizable Continuum Model: Theory and application to ground and excited-state polarizabilities of para-nitroaniline in solution. *J. Chem. Phys.*, 119:5818–5827, 2003.
- [25] R. Cammi, L. Frediani, B. Mennucci, and J. Tomasi. Calculation of nonlinear optical susceptibilities of pure liquids within the Polarizable Continuum Model: the effect of the macroscopic nonlinear polarization at the output frequency. *J. Mol. Structure-theochem*, 633:209–216, 2003.
- [26] R. Cammi, L. Frediani, B. Mennucci, J. Tomasi, K. Ruud, and K. V. Mikkelsen. A second-order, quadratically convergent Multiconfigurational Self-Consistent Field Polarizable Continuum Model for equilibrium and nonequilibrium solvation. *J. Chem. Phys.*, 117:13–26, 2002.
- [27] L. Frediani, C. S. Pomelli, and J. Tomasi. n-alkyl alcohols at the water/vapour and water/benzene interfaces: a study on phase transfer energies. *Phys. Chem. Chem. Phys.*, 2:4876–4883, 2000.
- [28] Luca Frediani, Eirik Fosgaard, Tor Flå, and Kenneth Ruud. Fast numerical algorithms for applying integral-operators in higher dimensions. Submitted.