LUCA FREDIANI

PERSONAL INFORMATION

Born in Italy, 6 January 1975

email luca.frediani@uit.no

website www.ctcc.no/people/senior-scientists/luca

phone (W) +47 776 44082 · (M) +47 47 323 585

WORK EXPERIENCE

2007–Present Associate professor, University of Tromsø

UiT, Tromsø

Developed a Multiwavelet code for accurate DFT calculations, wrote a standalone software module for continuum solvation calculations, developed an integrated QM/MM/PCM formalism, responsible for teaching several physical chemistry courses (bachelor, master and PhD level), supervised one master student (graduated in 2009) and two PhD students as main supervisor (graduated respectively in 2012 and 2014). Currently main supervisor of two additional PhD students. Youngest senior member of the Centre for Theoretical and Computational Chemistry (CTCC).

2005-2007 Postdoctoral fellow, University of Tromsø

Implemented solvent effect on cubic response properties at the DFT and MCSCF level. Implemented a Poisson solver using Multiwavelets.
Supervisor: Prof. Kenneth Ruud kenneth.ruud@uit.no

2004-2005 Postdoctoral fellow, KTH — Stockholm

KTH, Stockholm

Implemented solvent effect on quadratic response properties at DFT and MCSCF level.
Supervisor: Prof. Hans Ågren agren@theochem.kth.se

EDUCATION

2001-2004 University of Parma, Italy

PhD in Physical Chemistry

Thesis advisor: Prof. Roberto Cammi roberto.cammi@unipr.it

1994-2000 University of Pisa, Italy

Master in Chemistry

Thesis advisor: Prof. Jacopo Tomasi tomasi@dcci.unipi.it

1994-2000 Scuola Normale Superiore, Pisa, Italy

Chemistry major

Supervisor: Prof. Jacopo Tomasi tomasi@dcci.unipi.it

OTHER INFORMATION

Grants and awards

2014 · Conference grant, University of Tromsø (100.000NOK)

2014 · Educational grant, RESULT, University of Tromsø (100.000NOK): introduction of IT methods in Physical Chemistry

2009 · Young researcher prize, University of Tromsø (50.000NOK)

2008 · Research grant from Tromsø forskningsstiftelse (4.310.000 NOK): *"There is plenty to investigate at the surface: modeling of molecular properties at surfaces and interfaces*

2007 · Educational grant from UiT to establish a wavelet course for chemistry and physics (30.000 NOK).

2002 · Young researcher grant, University of Parma (4000€)

Early achievements track record

1. Youngest senior member of the Centre for Theoretical and Computational Chemistry (NFR-funded centre of excellence).

2. Developed and implemented the first multiwavelet code for all-electron Density Functional Theory calculations in Europe
3. Developed and implemented the first standalone module for solvation effect in quantum chemistry calculations with PCM. The module is currently interfaced with four different Quantum Chemistry softwares: Dalton, Dirac, LSDalton and PSI4.
4. Developed the first method to perform linear response calculation by making use of a layered QM/MM/PCM approach.
5. Received the young investigator award from The University of Tromsø as the best young scientist (below 35) in 2009.
6. I have published 37 articles and a book chapter. In 7 of them I am first author, corresponding in 18, and last author in 6 of them. The articles as first author are mostly from my PhD studies and my postdoc years. I have been often corresponding author during my postdoc years, which demonstrate achieved independence. Lately I have often been last author, which demonstrates the ability to lead scientific research.
7. I have an h-index of 18 (source: Google Scholar, Son ept 29 2015), and more than 1000 citations overall.

Teaching experience

1. General Chemistry (KJE-1001, UiT). Lecturer
2. Theoretical chemistry and spectroscopy (KJE-2001, UiT). Course responsible and Lecturer
3. Quantum Chemistry (KJE-3101, UiT). Course responsible and Lecturer
4. Computational chemistry (KJE-3102, UiT). Course responsible and Lecturer
5. Quantum chemistry methods (KJE-3103, UiT). Course responsible and Lecturer
6. Wavelet methods in physics and chemistry (MAT-8204, UiT). Course responsible and lecturer

Latest Conferences and meetings

2015 · NMQC-Tromsø *A voyage from molecules to materials with numerical methods for quantum chemistry*, Main orgainizer.

2014 · FemEx-Oslo *Promoting Female Excellence in Theoretical and Computational Chemistry*, Invited talk.

2012 · International Conference in Quantum Chemistry, Poster presentation

2011 · Cecam Workshop "New QM/MM opportunities for in silico macromolecular photochemistry", Lyon, France. Invited talk.

2009 · Conference "DFT09", Lyon, France, Poster presentation.

2008 · "XIV European Seminar on Computational Methods in Quantum Chemistry", Elba, Italy. Invited talk.

2008 · Workshop "Numerical methods in Density Functional Theory" Berlin, Germany. Invited talk.

Languages

Italian	·	Mother tongue
English, Norwegian	·	Fluent
Swedish, German	·	Basic

Programming skills

C, C++, Fortran (advanced)
Python, Autotools, Perl, Cmake (basic)

Interests

Hiking · Skiing · Running · Diving · Flute playing · Carpentry

References

Prof. Kenneth Ruud kenneth.ruud@uit.no
Prof. Arne Smalås arne.smalas@uit.no

September 29, 2015

PUBLICATIONS

[1] S.-R. Jensen, J. Juseluis, A. Durdek, T. Flå, P. Wind, and L. Frediani, "Accurate atomization energies with density functional theory and multiwavelets.", Manuscript in Preparation.

[2] S.-R. Jensen, P. Wind, J. Juselius, T. Flå, D. Jonsson, and L. Frediani, "Magnetic response properties at the basis set limit with multiwavelets", Manuscript in preparation.

[3] K. Mozgawa, R. Di Remigio, H. Cao, V. Weijo, and L. Frediani, "Electrostatic solvation at sphericical diffuse surfaces and interfaces", Manuscript in Preparation.

[4] R. Di Remigio, R. Bast, and L. Frediani, "4-Component Relativistic Calculations in Solution with the Polarizable Continuum Model of Solvation: Theory, Implementation and Application to the Group 16 . . . ", The Journal of Physical Chemistry (2014) 10.1021/jp507279y.

[5] A. Durdek, S. R. Jensen, J. Juselius, P. Wind, T. Flå, and L. Frediani, "Adaptive order polynomial algorithm in a multi-wavelet representation scheme", Applied Numerical Mathematics (2014).

[6] K. H. Hopmann, L. Frediani, and A. Bayer, "Iridium-PHOX-Mediated Alkene Hydrogenation: Isomerization Influences the Stereochemical Outcome", Organometallics **33**, 2790–2797 (2014).

[7] S. R. Jensen, J. Juselius, A. Durdek, T. Flå, P. Wind, and L. Frediani, "Linear scaling Coulomb interaction in the multiwavelet basis, a parallel implementation", Int. J. Model. Simul. Sci. Comput., 1441003 (2014).

[8] K. Mozgawa, B. Mennucci, and L. Frediani, "Solvation at Surfaces and Interfaces: A Quantum-Mechanical/Continuum Approach Including Nonelectrostatic Contributions", The Journal of Physical Chemistry C **118**, 4715–4725 (2014).

[9] K. Aidas, C. Angeli, K. L. Bak, V. Bakken, R. Bast, L. Boman, O. Christiansen, R. Cimiraglia, S. Coriani, P. Dahle, E. K. Dalskov, U. Ekström, T. Enevoldsen, J. J. Eriksen, P. Ettenhuber, B. Fernández, L. Ferrighi, H. Fliegl, L. Frediani, K. Hald, A. Halkier, C. Hättig, H. Heiberg, T. Helgaker, A. C. Hennum, H. Hettema, E. Hjertenaes, S. Høst, I.-M. Høyvik, M. F. Iozzi, B. Jansik, H. J. A. Jensen, D. Jonsson, P. Jorgensen, J. Kauczor, S. Kirpekar, T. Kjaergaard, W. Klopper, S. Knecht, R. Kobayashi, H. Koch, J. Kongsted, A. Krapp, K. Kristensen, A. Ligabue, O. B. Lutnaes, J. I. Melo, K. V. Mikkelsen, R. H. Myhre, C. Neiss, C. B. Nielsen, P. Norman, J. Olsen, J. M. H. Olsen, A. Osted, M. J. Packer, F. Pawlowski, T. B. Pedersen, P. F. Provasi, S. Reine, Z. Rinkevicius, T. A. Ruden, K. Ruud, V. V. Rybkin, P. Sałek, C. C. M. Samson, A. S. de Merás, T. Saue, S. P. A. Sauer, B. Schimmelpfennig, K. Sneskov, A. H. Steindal, K. O. Sylvester-Hvid, P. R. Taylor, A. M. Teale, E. I. Tellgren, D. P. Tew, A. J. Thorvaldsen, L. Thøgersen, O. Vahtras, M. A. Watson, D. J. D. Wilson, M. Ziolkowski, and H. Agren, "The Dalton quantum chemistry program system", WIREs Comput Mol Sci, n/a–n/a (2013).

[10] M. T. P. Beerepoot, A. H. Steindal, J. Kongsted, B. O. Brandsdal, L. Frediani, K. Ruud, and J. M. H. Olsen, "A polarizable embedding DFT study of one-photon absorption in fluorescent proteins", Phys Chem Chem Phys **15**, 4735–4743 (2013).

[11] L. Frediani, E. Fossgaard, T. Flå, and K. Ruud, "Fully adaptive algorithms for multivariate integral equations using the non-standard form and multiwavelets with applications to the Poisson and bound-state Helmholtz kernels in three dimensions", Mol Phys **111**, 1143–1160 (2013).

[12] A. H. Steindal, J. M. H. Olsen, L. Frediani, J. Kongsted, and K. Ruud, "Parallelization of the polarizable embedding scheme for higher-order response functions", Mol Phys **110**, 2579–2586 (2012).

[13] A. H. Steindal, J. M. H. Olsen, K. Ruud, L. Frediani, and J. Kongsted, "A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein.", Phys Chem Chem Phys **14**, 5440–5451 (2012).

[14] A. H. Steindal, K. Ruud, L. Frediani, K. Aidas, and J. Kongsted, "Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method", Journal of Physical Chemistry B **115**, 3027–3037 (2011).

[15] L. Ferrighi, L. Frediani, and K. Ruud, "Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model.", J Chem Phys **132**, 024107 (2010).

[16] V. Weijo, B. Mennucci, and L. Frediani, "Toward a General Formulation of Dispersion Effects for Solvation Continuum Models", J Chem Theory Comput **6**, 3358–3364 (2010).

[17] V. Weijo, M. Randrianarivony, H. Harbrecht, and L. Frediani, "Wavelet Formulation of the Polarizable Continuum Model", J Comput Chem **31**, 1469–1477 (2010).

[18] S. Corni and L. Frediani, "Molecules at surfaces and interfaces", in *Continuum solvation models in chemical physics: from theory to applications*, edited by B. Mennucci and R. Cammi (Wiley, 2008), p. 300.

[19] H. Solheim, L. Frediani, K. Ruud, and S. Coriani, "An IEF-PCM study of solvent effects on the Faraday B term of MCD", Theoretical Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) **119**, 231–244 (2008).

[20] L. Ferrighi, L. Frediani, and K. Ruud, "Two-photon absorption of [2.2] paracyclophane derivatives in solution: A theoretical investigation", J Chem Phys **127**, 244103 (2007).

[21] L. Ferrighi, L. Frediani, and K. Ruud, "Degenerate four-wave mixing in solution by cubic response theory and the polarizable continuum model", Journal of Physical Chemistry B **111**, 8965–8973 (2007).

[22] 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** (2007) 10.1063/1.2787527.

[23] K. Zhao, L. Ferrighi, L. Frediani, C.-K. Wang, and Y. Luo, "Solvent effects on two-photon absorption of dialkylamino substituted distyrylbenzene chromophore", J Chem Phys **126** (2007) 10.1063/1.2740641.

[24]L. Bondesson, L. Frediani, H. Agren, and B. Mennucci, "Solvation of N-3(-) at the water surface: The Polarizable Continuum Model approach", Journal of Physical Chemistry B **110**, 11361–11368 (2006).

[25]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**, 267–272 (2006).

[26]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**, 154112 (2006).

[27]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** (2006) 10.1063/1.2404661.

[28]M. Pecul, E. Lamparska, 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).

[29]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).

[30]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).

[31]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).

[32]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 Chemistry Accounts: Theory, Computation, and Modeling (Theoretica Chimica Acta) **111**, 66–77 (2004).

[33]L. Frediani, B. Mennucci, and R. Cammi, "Quantum-mechanical continuum solvation study of the polarizability of halides at the water/air interface", Journal of Physical Chemistry B **108**, 13796–13806 (2004).

[34]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).

[35]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 Comput Chem **25**, 375–385 (2004).

[36]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).

[37]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 Struc-Theochem **633**, 209–216 (2003).

[38]K. Ruud, L. Frediani, R. Cammi, and B. Mennucci, "Solvent effects on the indirect spin-spin coupling constants of benzene: The DFT-PCM approach", International Journal of Molecular Sciences **4**, 119–134 (2003).

[39]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).

[40]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).