Lara Ferrighi

Curriculum vitae updated on September 28, 2009

Personal details

- Full name: Lara Ferrighi
- Date of birth: June 13, 1979
- Nationality: Italian
- Work address: Department of Physics and Astronomy, University of Århus, Ny Munkegade, DK-8000 Århus C
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Education

March 2008 : PostDoc at the department of Physics and Astronomy, University of Århus. The TPSS and M06L Meta-GGA functionals, containing information on the kinetic energy, have been implemented in the GPAW code. The new implementation has been used to calculate the stability of Gold clusters, with positive and negative charge.

November 2007 : Defence of the Ph.D. thesis "Linear and Nonlinear properties of molecules in solution"

2004-2008 : Ph.D. student at University of Tromsø under the supervision of Prof. Kenneth Ruud, Department of Chemistry. The main subject of my Ph.D. thesis is related to solvent effects on molecular properties. The Polarizable Continuum Model (PCM) has been applied both to first and second nonlinear optical properties as well as to magnetic properties. An extension to the PCM code in order to calculate third order properties has been developed and implemented during the Ph.D. period within the Dalton program.

July 16, 2003 Degrees in Theoretical Chemistry, 110/110 *cum laude* discussing the master thesis "Study on electronic transitions in organic molecules, containing more than one chromophore, using localized orbitals" under the supervision of Prof. Renzo Cimiraglia and Dr. Celestino Angeli.

1998–2003 University courses in Chemistry at the University of Ferrara, Italy

1993–1998 Secondary school at Liceo Scientifico Statale "P. Paleocapa" of Rovigo, Italy

Partecipation in schools and conferences

May 14-15, 2009 "Cost Action D41 Inorganic Oxides: Surfaces and Interfaces", Göteborg (Sweden)

October 16-18, 2008 "Cost Action D41 Inorganic Oxides: Surfaces and Interfaces", Barcelona (Spain)

August 18-29, 2008 "The CAMD Summer School on Electronic Structure Theory and Materials Design " DTU (Copenhagen), Denmark

June 5-6, 2008 " Workshop on density-functional calculations in real-space/Time-dependent density-functional theory with GPAW" Espoo, Finland

November 9-11, 2007 "Norwegian Theoretical Chemistry-From molecules to nanostructures", Trondheim, Norway

October 18, 2007 "the 18th Norwegian Chemical Society meeting", Lilletrøm, Norway

September 2-15, 2007 "European Summerschool in Quantum Chemistry 2007", Palermo, Italy

May 29-June 3 2007 "Molecular Quantum Mechanics - Analytic Gradients and Beyond", Budapest, Hungary

May 6 2006 "Experiment-oriented quantum chemistry tools for spectroscopies based on electric, magnetic, and vibrational phenomena", COST 26 meeting, Stockholm, Sweden

May 4-5 2006 Swedish Theoretical Chemistry, Albanova University Center, Stockholm, Sweden

October 20-27, 2005 International Conference of Computational Methods in Sciences and Engineering, Loutraki, Greece

April 2005 COST 26 action meeting, Pisa, Italy

June 28-29, 2005 Quantum chemistry SUP meeting, Bergen, Norway

November 09-11, 2004 Quantum-chemistry SUP meeting, Oslo, Norway

September 17-20, 2004 Workshop Italian-Norwegian-Swedish Workshop on Quantum Molecular Sciences, Tromsø, Norway

July 24-29, 2004 Molecular Quantum Mechanics: The No Nonsense Path to Progress, St. John's College, Cambridge, England

June 20 - July 2, 2004 "The 8th Sostrup Summer School: Quantum Chemistry and Molecular Properties" Århus, Denmark

Lectures and poster presentation

Oral Presentation "2D-3D transition for positive and negative Gold clusters. A kinetic energy density functional study", Cost Meeting Göteborg (Sweden)

Poster L. Ferrighi:"Meta-GGA functionals in GPAW code": Cost meeting, Barcelona, Spain

Oral Presentation "Cubic Response Theory in the Polarizable Continuum Model: framework, theory and applications" Norwegian Theoretical Chemistry-From molecules to nanostructures, Trondheim, Norway

Poster L. Ferrighi: "Degenerate Four-Wave Mixing in solution by Cubic Response Theory and the Polarizable Continuum Model" Budapest, Hungary

Oral Presentation "Second-Order NLO properties of Green Fluorescent Protein: structure and effects of the surroundings", Department of Chemistry, Bergen, Norway

Poster L. Ferrighi and H. Solheim: "Solvent effect on optical activity: Rotatory Power and Magnetic Circular Dichroism" Swedish Theoretical Chemistry, Albanova University Center, Stockholm, Sweden

Oral Presentation L. Ferrighi: "Solvent effect on molecular properties: the hyperpolarizability", Dipartimento di Scienze Chimiche, Trieste, Italy

Oral Presentation L. Ferrighi: " Comparison between theoretical and experimental hyperpolarizabilities: the PCM model". Quantum chemistry SUP meeting, Bergen, Norway

Oral Presentation L. Ferrighi: "Solvent effects on hyperpolarizability in conjugated polyenes and on magnetizability in amino acids". Quantum-chemistry SUP meeting, Oslo, Norway

Poster L. Ferrighi: "Study on electronic transitions in organic molecules, containing more than one chromophore, using localized orbitals" Molecular Quantum Mechanics: The No Nonsense Path to Progress, St. John's College, Cambridge, England

Teaching experience

Spring 2006 and 2007, Autumn 2007 Seminar lectures for Computational Chemistry KJE-3102

Spring 2005 Seminar lectures for Quantum Chemical Methods KJE-3103

Autumn 2004, 2005 and 2007 Seminar lectures for Inorganic Chemistry KJE-1004

Miscellaneous

September 2004 10 days visiting researcher of L. Frediani at Albanova University Center, Stockholm, Sweden

April 2005 one week visiting researcher of S. Coriani at Dipartimento di Scienze Chimiche, Trieste, Italy

August-December 2006 4 months visiting researcher of B. Champagne at Laboratoire de Chimie Theorique Applique Facultes Universitaires Notre-Dame de la Paix, NAMUR, Belgium

Other informations

Informatic knowledge: Experience with linux and open-source software, and use of the principal software in the Windows environment. Basic programing skills in Fortran, C and Python.

Languages: Italian (mother tongue), fluent written and spoken english, basic knowledge of norwegian.

References

Prof. Kenneth Ruud , Centre for Theoretical and Computational Chemistry, University of Tromsø, N-9037 Tromsø, Norway
email: Kenneth.Ruud@chem.uit.no

Prof. Celestino Angeli , Dipartimento di Chimica, Universitegli studi di Ferrara, Ferrara, Italy
email: cele@icbe62.unife.it

Prof. Benoit Champagne Laboratoire de Chimie Theorique Appliquee Facultes Universitaires Notre-Dame de la Paix B-5000 NAMUR Belgium
email: benoit.champagne@fundp.ac.be

List of publications

1. 2D-3D transition for cationic and anionic Gold clusters. A kinetic energy density functional study
   L. Ferrighi, G. Madsen, B. Hammer
   J. Am. Chem. Soc. 131 (30) 10605 (2009)

2. Excited state polarizability by means of Cubic Response and the Polarizable Continuum Model
   L. Ferrighi, L. Frediani and K. Ruud
   Submitted

3. Analytic *ab initio* calculations of Coherent anti-Stokes Raman Scattering (CARS) for polyaromatic hydrocarbons
   A. J. Thorvaldsen, L. Ferrighi, K. Ruud, H. Ågren, P. Jørgensen and S. Coriani
   Phys. Chem. Chem. Phys 11 (13) 2293 (2008)

4. Solvent effects on Three-Photon Absorption of a symmetric Charge-Transfer Molecule
N. Lin, L. Ferrighi, X. Zhao, K. Ruud, A. Rizzo, Y. Luo
J. Phys. Chem. B 1520-6106 (2008)

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

6. Extended Viologen, a Diradical Species Exhibiting Large Second Hyperpolarizability
L. Ferrighi, E. Botek, M. Nakano, R. Kishi, S. Ohta, M. Nate, H. Takahanasci, T. Kubo, K. Kamada, K. Ohta and B. Champagne
In preparation

7. Second-harmonic generation in GFP-like proteins
I. Asselberghs, C. Flors, L. Ferrighi, E. Botek, B. Champagne, H. Mizuno, R. Ando, A. Miyawaki, J. Hofkens, M. Van der Auweraer, K. Clays1.
J. Am. Chem. Soc., 130 (46) 15713 (2008)

8. Solvent Effects on Two-Photon Absorption of Dialkylamino Substituted Distyrylbenzene Chromophore
K. Zhao, L. Ferrighi, L. Frediani, C. Wang, and Y. Luo
J. Chem. Phys. 126 204509 (2007)

9. Degenerate Four-Wave Mixing in solution by Cubic Response Theory and the Polarizable Continuum Model
L. Ferrighi, L. Frediani and K. Ruud
J. Phys. Chem. B 1520-6106 (2007)

10. Parallelization of the integral equation formulation of the polarizable continuum model for higher-order response functions
L. Ferrighi, L. Frediani, E. Fossgaard and K. Ruud
J. Chem. Phys., 125 154112, (2006)

11. Density-functional-theory study of the electric-field-induced second harmonic generation (EFISHG) of push-pull phenylpolyenes in solution
L. Ferrighi, L. Frediani, C. Cappelli, P. Salek, H. Ågren, T. Helgaker and K. Ruud
Chem. Phys. Lett., 425 267-272 (2006)

12. Solvent effects on the conformational distribution and optical rotation of gamma-methyl paraconic acids and esters
S. Coriani, A. Baranowska, L. Ferrighi, C. Forzato, D. Marchesan, P. Nitti, G. Pitacco, A. Rizzo ans K. Ruud
Chirality, 18 357-369 (2006)

13. Developments in the n-electron valence state perturbation theory
C. Angeli, S. Borini, A. Cavallini, M. Cestari, R. Cimiraglia, L. Ferrighi, M. Sparta
Int. J. Quant. Chem., 106 686-691 (2006)

14. Gauge-origin-independent magnetizabilities of solvated molecules using the polarizable continuum model
L. Ferrighi, D. Marchesan, K. Ruud, L. Frediani and S. Coriani
J. Chem. Phys., 123 (2005)

15. Second-harmonic generation of solvated molecules using multiconfigurational self-consistent-field quadratic response theory and the polarizable continuum model
L. Frediani, H. Ågren, L. Ferrighi and K. Ruud
J. Chem. Phys., 123 (2005)

16. A CASSCF theoretical study of the vibrational frequencies and structure of formaldehyde, acetaldehyde and acetone valence excited states
C. Angeli, S. Borini, L. Ferrighi, R. Cimiraglia
J. Mol. Struc. THEOCHEM, 718 55-69 (2005)

17. Ab initio n-electron valence state perturbation theory study of the adiabatic transitions in carbonyl molecules: Formaldehyde, acetaldehyde, and acetone
C. Angeli, S. Borini, L. Ferrighi, R. Cimiraglia
J. Chem. Phys., 122 (2005)