Franco Egidi, PhD

Personal

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Summary

I am an Italian Chemistry PhD and I did my Graduate studies at the Scuola Normale Superiore in Pisa (Italy). The topic of my PhD work has been the development of theoretical and computational methods for the calculation of spectroscopic properties of molecular systems in solution, particularly in the case mixed electronic-vibrational spectroscopies. During my PhD I have also had experience as an assistant lecturer, and have often mentored undergraduate and younger graduate students with their research work. After my PhD I moved to the University of Washington to work as a PostDoc doing research focused on the development of methods for the treatment of spin-dependent relativistic effects in the simulation of excited states of molecular systems, before going back to Pisa to continue my reasearch as a PostDoc.

Work & Education

Period	September 2016 — Present
Employer	Scuola Normale Superiore, Pisa (Italy)
Job Title	Research Associate (PostDoc)
Period	January 2015 — September 2016
Employer	University of Washington, Seattle (WA)
Job Title	Research Associate (PostDoc)
Period	November 2011 — December 2014
Degree	PhD in Chemistry
University	Scuola Normale Superiore, Pisa (Italy)
Period	October 2006 — July 2011
Degree	Bachelor's and Master's degree in Chemistry
University	University of Pisa, Pisa (Italy)

Languages

Italian	Mother tongue.
English	Proficient.

Research & Work Experience

Personal Skills

During my university and research career I have developed extensive research skills in the field of Physical Chemistry. My research work included a heavy amount of programming in different languages, including Fortran (especially within the Gaussian09 quantum chemistry package), MatLab, Python, and Shell scripting. I am comfortable using both Windows and Linux operating systems. For my research activity I routinely use the Office suite of programs, the LaTeX typesetting system, and numerous molecular editors and programs for elaborating and plotting data. In addition, I have been involved first-hand in the preparation of research papers and grant applications, and I have attended numerous international scientific conferences, presenting my work with posters and

talks. As part of my research program I have had the opportunity to help and mentor younger students, and I have also been involved in the teaching of a computational chemistry class as a Teaching Assistant (TA). Finally, during Graduate school I have been involved in the writing and grading of the Undergraduate admission exams for my University (the Scuola Normale Superiore), and I have had the opportunity to participate in orientation events organized by the University for perspective students, which included mentoring and giving a lecture explaining the nature of the research conducted by my group.

Publications

1. F. Egidi, F. Trani, P. Ballone, V. Barone, W. Andreoni, "Low-lying Electronic Excitations of a Water-Soluble Bodipy: from the Gas Phase to the Solvated Molecule" *Theo. Chem. Acc.* (2016) Just Accepted

2. D. Williams-Young, F. Egidi, X. Li, "Relativistic Two-Component Particle-Particle Tamm-Dancoff Approximation" *J. Chem. Theory Comput.* (2016) In press

3. J. Goings, J. Kasper, F. Egidi, S. Sun, X. Li, "Real Time Propagation of the Exact Two Component Time-Dependent Density Functional Theory" *J. Chem. Phys.* 145 (2016) 104107

4. F. Egidi, J. Goings, M. Frisch, X. Li, "Direct Atomic-Orbital-Based Relativistic Two-Component Linear Response Method for Calculating Excited-State Fine Structures" *J. Chem. Theory Comput.* 12 (2016) 3711

5. P. Lestrange, F. Egidi, X. Li, "The Consequences of Improperly Describing Oscillator Strengths Beyond the Electric Dipole Approximation" *J. Chem. Phys.* 143 (2015) 234103

6. F. Egidi, C. Cappelli, "Calculation of Molecular Properties in Solution" *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering* (2015)

7. L. Vidal, F. Egidi, V. Barone, C. Cappelli, "Origin invariance in vibrational resonance Raman optical activity" *J. Chem. Phys.* 142 (2015) 174101

8. E. Benassi, F. Egidi, V. Barone, "A General Strategy for Computing Non-Linear Optical Properties of Large Neutral and Cationic Organic Chromophores in Solution" *J. Phys. Chem. B* 119 (2015) 3155

9. F. Egidi, R. Russo, I. Carnimeo, A. D'Urso, G. Mancini, C. Cappelli, "The Electronic Circular Dichroism of Nicotine in Aqueous Solution: A Test Case for Continuum and Mixed Explicit-Continuum Solvation Approaches" *J. Phys. Chem. A* 119 (2015) 5396

10. F. Egidi, I. Carnimeo, C. Cappelli, "Optical rotatory dispersion of methyloxirane in aqueous solution: assessing the performance of density functional theory in combination with a fully polarizable QM/MM/PCM approach" *Opt. Mater. Express* 5 (2015) 196

11. F. Egidi, M. Segado, H. Koch, C. Cappelli, V. Barone, "A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule" *J. Chem. Phys.* 141 (2014) 224114

12. D. Licari, A. Baiardi, M. Biczysko, F. Egidi, C. Latouche, V. Barone, "Implementation of a Graphical User Interface for the Virtual Multifrequency Spectrometer: The VMS-Draw Tool" *J. Comput. Chem.* 36 (2014) 321

13. F. Egidi, T. Giovannini, M. Piccardo, J. Bloino, C. Cappelli, V. Barone, "Stereoelectronic, Vibrational, and Environmental Contributions to Polarizabilities of Large Molecular Systems: A Feasible Anharmonic Protocol" *J. Chem. Theory Comput.* 10 (2014) 2456

14. F. Egidi, J. Bloino, C. Cappelli, V. Barone, "A Robust and Effective Time-Independent Route to the Calculation of Resonance Raman Spectra of Large Molecules in Condensed Phases with the Inclusion of Duschinsky, Herzberg–Teller, Anharmonic, and Environmental Effects" *J. Chem. Theory Comput.* 10 (2014) 346

15. M. Lessi, C. Manzini, P. Minei, L.A. Perego, J. Bloino, F. Egidi, V. Barone, A. Pucci, F. Bellina, "Synthesis and Optical Properties of Imidazole-Based Fluorophores having High Quantum Yields" *ChemPlusChem* 79 (2014) 366

16. F. Egidi, J. Bloino, C. Cappelli, V. Barone, "Development of a Virtual Spectrometer for Chiroptical Spectroscopies: The Case of Nicotine" *Chirality* 25 (2013) 701

17. V. Barone, M. Biczysko, F. Egidi, C. Puzzarini, "Accurate structure, thermodynamics, and spectroscopy of medium-sized radicals by hybrid coupled cluster/density functional theory approaches: The case of phenyl radical" *J. Chem. Phys.* 138 (2013) 234303

18. F. Lipparini, F. Egidi, C. Cappelli, V. Barone, "The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?" *J. Chem. Theory Comput.* 9 (2013) 1880

19. F. Egidi, J. Bloino, C. Cappelli, V. Barone, J. Tomasi, "Tuning of NMR and EPR Parameters by Vibrational Averaging and Environmental Effects: an Integrated Computational Approach" *Mol. Phys.* 111 (2013) 1345

20. F. Egidi, J. Bloino, V. Barone, C. Cappelli, "Toward an Accurate Modeling of Optical Rotation for Solvated Systems: Anharmonic Vibrational Contributions Coupled to the Polarizable Continuum Model" *J. Chem. Theory Comput.* 8 (2012) 585

Conferences

- Theory and Applications of Computational Chemistry (TACC2016). August 2016, Seattle (WA). Oral presentation.
- Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST). June 2016, Telluride (CO). Poster presentation.
- International Chemical Congress of Pacific Basin Societies (PacifiChem). December 2015, Honolulu (HA). Oral presentation.
- European Seminar on Computational Methods in Quantum Chemistry. September 2014, Houffalize (Belgium). Poster presentation.
- Solutions for Solvation International Workshop. August 2014, Pisa (Italy). Oral presentation.
- Winter Modeling Workshop. November 2012, Pisa (Italy). Poster presentation.
- International Meeting on Atomic and Molecular Physics and Chemistry. September 2012, Pisa (Italy). Oral presentation.
- Vibrational Optical Activity: Interplay of Theory and Experiment. September 2012, Pisa (Italy). Poster presentation.

Schools

- 12th Sostrup Summer School in Quantum Chemistry and Molecular Properties. July 2012, Himmelbjerget (Denmark).
- Winter School in Theoretical Chemistry. December 2011, Helsinki (Finland).

References

- Prof Vincenzo Barone (vincenzo.barone@sns.it), Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa (PI), Italy.
- Prof Xiaosong Li (xsli@uw.edu), University of Washington, 305 Bagley Hall, 98195 Seattle (WA), USA.