CURRICULUM VITAE

Francesco Evangelista, Ph.D.

Assistant Professor, Emory University

Contact Information

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Education

2005–2008 | *Doctor of Philosophy*, **University of Georgia**, Athens, Georgia, USA
Dissertation topic: Multireference coupled cluster theory
Dissertation advisor: Professor Henry F. Schaefer

1999–2004 | *Diploma*, **Scuola Normale Superiore di Pisa**, Pisa, Italy
Thesis topic: Radicals derived from adenine and adenosine
Diploma advisor: Professor Benedetta Mennucci

1999–2004 | *Bachelor of Science*, **University of Pisa**, Pisa, Italy
Thesis topic: Dynamics of the internal conversion of ethylene
Thesis advisor: Professor Maurizio Persico

Professional Experience

2013–Present | *Assistant Professor*, **Emory University**, Atlanta, GA , USA

2011–2013 | *Postdoctoral Associate*, **Yale University**, New Haven, CT, USA
Topic: The role of electronic excitations on chemical reaction dynamics at metal, semiconductor, and nanoparticle surfaces
Advisor: Professor John C. Tully

2009–2011 | *Postdoctoral Scholar and Alexander von Humboldt Fellow*, **University of Mainz**, Mainz, Germany
Topic: Development and application of alternative single-reference and internally contracted multireference coupled cluster theories
Host: Professor Jürgen Gauss

Fellowships

2010–2011	Alexander von Humboldt Junior Fellowship for Postdoctoral Researchers
2005–2008	Enrico Fermi Fellowship, Center for Computational Chemistry, University of Georgia
1999–2004	Full Scholarship, Scuola Normale Superiore di Pisa

Academic Honors and Awards

2005	Graduate Student Poster Award, 2005 Annual Meeting of the Southeast Theoretical Chemistry Association
2003	Summer Undergraduate Research Fellowship, Center for Computational Chemistry, University of Georgia
1999	Prize “Per un futuro intelligente” of the Italian Federation of the Chemical Industry (Federchimica)
1999	Gold Medal, XXXI International Chemistry Olympiads, Bangkok, Thailand
1998	Silver Medal, XXX International Chemistry Olympiads, Melbourne, Australia

Teaching Experience

2008	Advanced Quantum Chemistry, Teaching Assistant, University of Georgia
2006	Modern Organic Chemistry Laboratory II, Teaching Assistant, University of Georgia
2005–2008	Summer Undergraduate Research Program, Instructor, University of Georgia

Scientific Collaborators

Doctor Andreas Köhn	University of Mainz, Germany
Professor Jürgen Gauss	University of Mainz, Germany
Professor Paul v. R. Schleyer	University of Georgia, USA
Professor Debashis Mukherjee	Raman Center for Atomic, Molecular and Optical Sciences Indian Association for the Cultivation of Science, Kolkata, India

Publications

[1] **F. A. Evangelista**, M. Hanauer, A. Köhn, and J. Gauss *A sequentially transformed internally contracted multireference coupled cluster approach*, (in preparation).

[2] **F. A. Evangelista** and J. Gauss, *On the role of generalized normal ordering and many-body conditions in internally contracted multireference coupled cluster approaches: A second-order perturbative analysis*, (in preparation).

[3] **F. A. Evangelista** and J. Gauss, *On the approximation of the similarity-transformed Hamiltonian in single-reference and multireference coupled cluster theory*, *Chem. Phys.* DOI:10.1016/j.chemphys.2011.08.006 (2011).

[4] **F. A. Evangelista**, *Alternative single-reference coupled cluster approaches for multireference problems: The simpler, the better*, *J. Chem. Phys.* **134**, 224102 (2011).

[5] **F. A. Evangelista** and J. Gauss, *An orbital-invariant internally-contracted multireference coupled cluster approach*, *J. Chem. Phys.* **134**, 114102 (2011).

[6] **F. A. Evangelista** and J. Gauss, *Insights into the orbital invariance problem in state-specific multireference coupled cluster theory*, *J. Chem. Phys.* **133**, 044101 (2010).

[7] T. Lu, A. C. Simmonett, **F. A. Evangelista**, Y. Yamaguchi, D.-C. Fang, and H. F. Schaefer, *Low-lying triplet states of diphosphene and diphosphinylidene*, *J. Phys. Chem. A* **114**, 10850 (2010).

[8] Q. Cheng, A. C. Simmonett, **F. A. Evangelista**, Y. Yamaguchi, and H. F. Schaefer, *Characterization of the BNNO radical*, *J. Chem. Theory Comput.* **6**, 1915 (2010).

[9] **F. A. Evangelista**, E. Prochnow, J. Gauss, and H. F. Schaefer, *Perturbative triples corrections in state-specific multireference coupled cluster theory*, *J. Chem. Phys.* **132**, 074107 (2010).

[10] T.-C. Jagau, E. Prochnow, **F. A. Evangelista**, , and J. Gauss, *Analytic gradients for Mukherjee's multireference coupled-cluster method using two-configurational self-consistent-field orbitals*, *J. Chem. Phys.* **132**, 144110 (2010).

[11] J. I. Wu, **F. A. Evangelista**, and P. von Rague Schleyer, *Why are perfluorocyclobutadiene and some other $(CF)_q^n$ rings non-planar?*, *Org. Lett.* **12**, 768 (2010).

[12] Q. Cheng, **F. A. Evangelista**, A. C. Simmonett, Y. Yamaguchi, and H. F. Schaefer, *Water dimer radical cation: Structures, vibrational frequencies, and energetics*, *J. Phys. Chem. A* **113**, 13779 (2009).

[13] T. Lu, A. C. Simmonett, **F. A. Evangelista**, Y. Yamaguchi, and H. F. Schaefer, *Diphosphene and diphosphinylidene*, *J. Phys. Chem. A* **113**, 13227 (2009).

[14] E. Prochnow, **F. A. Evangelista**, H. F. Schaefer, W. D. Allen, and J. Gauss, *Analytic gradients for the state-specific multireference coupled cluster singles and doubles model*, *J. Chem. Phys.* **131**, 064109 (2009).

[15] **F. A. Evangelista**, A. C. Simmonett, H. F. Schaefer, D. Mukherjee, and W. D. Allen, *A companion perturbation theory for state-specific multireference coupled cluster methods*, *Phys. Chem. Chem. Phys.* **11**, 4728 (2009).

[16] **F. A. Evangelista**, A. C. Simmonett, W. D. Allen, H. F. Schaefer, and J. Gauss, *Triple excitations in state-specific multireference coupled cluster theory: Application of Mk-MRCCSDT and Mk-MRCCSDT-n methods to model systems*, *J. Chem. Phys.* **128**, 124104 (2008).

[17] J. C. Hargis, **F. A. Evangelista**, J. B. Ingels, and H. F. Schaefer, *Short intramolecular hydrogen bonds: Derivatives of malonaldehyde with symmetrical substituents*, *J. Am. Chem. Soc.* **130**, 17471 (2008).

[18] **F. A. Evangelista**, W. D. Allen, and H. F. Schaefer, *Coupling term derivation and general implementation of state-specific multireference coupled cluster theories*, *J. Chem. Phys.* **127**, 024102 (2007).

[19] A. C. Simmonett, **F. A. Evangelista**, and W. D. Allen, *In search of definitive signatures of the elusive NCCO radical*, *J. Chem. Phys.* **127**, 014306 (2007).

[20] **F. A. Evangelista**, W. D. Allen, and H. F. Schaefer, *High-order excitations in state-universal and state-specific multireference coupled cluster theories: Model systems*, *J. Chem. Phys.* **125**, 154113 (2006).

[21] **F. A. Evangelista** and H. F. Schaefer, *Hydrogen atom and hydride anion addition to adenine: Structures and energetics*, *ChemPhysChem* **7**, 1471 (2006).

[22] **F. A. Evangelista** and H. F. Schaefer, *Structures and energetics of adenosine radicals: (2'-dAdo-H)$^\bullet$*, *J. Phys. Chem. A* **108**, 10258 (2004).

[23] **F. A. Evangelista**, A. Paul, and H. F. Schaefer, *Radicals derived from adenine: Prediction of large electron affinities with a considerable spread*, *J. Phys. Chem. A* **108**, 3565 (2004).

Conference Lectures

September 8–12, 2013	"Adaptive quantum chemistry methods", *246th meeting of the American Chemical Society* (ACS 2013), Indianapolis, Indiana, USA.
July 2, 2013	"Three variations on single-reference coupled cluster theory", *ICQC Workshop: Coupled-Cluster theory and related techniques*. (ICQC 2012), Boulder, Colorado, USA.
July 17–22, 2011	"An orbital invariant internally-contracted multireference coupled cluster approach", *World Association of Theoretical and Computational Chemists* (WATOC 2011), Santiago de Compostela, Spain.
June 16–19, 2011	"An orbital invariant internally-contracted multireference coupled cluster approach", *European Seminar on Computational Methods in Quantum Chemistry* (ESCMQC11), Oscarsborg Fortress, Drøbak, Norway.
September 26–30, 2010	"Is internally-contracted multireference coupled cluster theory the way to go?", *46th Symposium on Theoretical Chemistry* (STC 2010), Münster, Germany.
February 24–March 2, 2010	"Recent developments in multireference coupled cluster theory", *Sanibel Symposium*, St. Simons Island, Georgia, USA.
September 14–19, 2008	"A perturbative triples correction for state-specific multireference coupled cluster theory", *World Association of Theoretical and Computational Chemists* (WATOC 2008), Sydney, Australia.
July 19–24, 2008	"Achieving accurate thermochemistry in state-specific multireference coupled cluster theory", *Sixth Congress of the International Society for Theoretical Chemical Physics* (ISTCP-VI 2008), Vancouver, Canada.
January 10–12, 2008	"Triple excitations in state-specific multireference coupled cluster theory", *Symposium on Atomic, Molecular and Optical Sciences & High Performance Computing: A Seamless Frontier*, Kolkata, India.

Scholarly Activities

Active reviewer for the following journals:

- The Journal of Chemical Physics
- Chemical Physics Letters
- ChemPhysChem
- Molecular Physics
- Theoretical Chemistry Accounts
- Journal of Computational Chemistry
- Canadian Journal of Chemistry

Active reviewer for the following funding institutions:

- American Chemical Society - Petroleum Research Fund

Professional Societies

American Chemical Society