Francesco A. Evangelista

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Contact Information

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Professional Experience

2013–Pres.	*Assistant Professor of Chemistry*, Emory University, Atlanta, Georgia
2011–2013	*Postdoctoral Associate*, Yale University, New Haven, Connecticut Advisor: Professor John C. Tully
2009–2011	*Alexander von Humboldt Fellow*, University of Mainz, Mainz, Germany Host: Professor Jürgen Gauss

Education

2005–2008	*Doctor of Philosophy*, University of Georgia, Athens, Georgia Dissertation advisor: Professor Henry F. Schaefer
1999–2004	*Diploma*, Scuola Normale Superiore di Pisa, Pisa, Italy *Bachelor of Science*, University of Pisa, Pisa, Italy Thesis advisor: Professor Maurizio Persico

Academic Honors, Awards, and Fellowships

2017	Dirac Medal, World Association of Theoretical and Computational Chemists (WATOC)
2016	Department of Energy Early Career Award
2016	National Science Foundation CAREER Award (*awarded but later withdrawn due to a conflict with the DOE Early Career Award*)
2016	Alfred P. Sloan Research Fellow
2010–2011	Alexander von Humboldt Junior Fellowship for Postdoctoral Researchers
1999–2004	Full Scholarship, Scuola Normale Superiore di Pisa
2005	Graduate Student Poster Award, 2005 Annual Meeting of the Southeast Theoretical Chemistry Association
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

2014–2017	Modern Techniques in Computational and Theoretical Chemistry (CHEM532, graduate), Emory University
2014–2017	Physical Chemistry I (CHEM331, undegraduate), Emory University
2016	Perspectives in Chemistry (CHEM-468W, undegraduate), Emory University

Outreach, Mentoring, and Synergistic Activities

Outreach	Contributed to *Decoding Nature's Puzzles*, a one-day outreach event that introduces 10–18 year old girls to coding and computer engineering. Gave a presentation entitled "Simulating Chemistry with a Computer" to groups of high-school students. In this talk I explain the objective and importance of computer simulations in science.
Mentoring	Mentored three undergraduate students (Momo Rutkin, Andy Zeng, Xiaobai Li), one of whom is now pursuing a PhD in Physical Chemistry at Yale University.
Professional	Organizer of the 2014 *Meeting of the Southeastern Theoretical Chemistry Association*, May 15–17, Atlanta, Georgia. This low cost regional meeting emphasized student participation trough contributed talks and poster presentations.
Coding	Developer of the open-source quantum chemistry packages Psi4 and Forte.

Publications (total = 42, h-index = 19, sum of the times cited = 1513)

Since starting independent career at Emory (1–17), Prior to Emory (18–42)

[1] C. Li and F. A. Evangelista, *Driven similarity renormalization group for excited states: A state-averaged perturbation theory*, *(accepted)* .

[2] W. D. Derricotte and F. A. Evangelista, *Localized Intrinsic Valence Virtual Orbitals as a Tool for the Automatic Classification of Core Excited States.*, *J. Chem. Theory Comput.* 13, 5984 (2017).

[3] J. M. Brockman, A. T. Blanchard, V. Pui-Yan, et al., *Mapping the 3D orientation of piconewton integrin traction forces.*, *Nat. Methods* 70, 2008 (2017).

[4] J. B. Schriber and F. A. Evangelista, *Adaptive Configuration Interaction for Computing Challenging Electronic Excited States with Tunable Accuracy.*, *J. Chem. Theory Comput.* 13, 5354 (2017).

[5] C. Li, P. Verma, K. P. Hannon, and F. A. Evangelista, *A low-cost approach to electronic excitation energies based on the driven similarity renormalization group*, *J. Chem. Phys.* 147, 074107 (2017).

[6] R. M. Parrish, L. A. Burns, D. G. A. Smith, et al., *Psi41.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability*, *J. Chem. Theory Comput.* 13, 3185 (2017).

[7] C. Li and F. A. Evangelista, *Driven similarity renormalization group: Third-order multireference perturbation theory*, *J. Chem. Phys.* 146, 124132 (2017).

[8] T. Zhang and F. A. Evangelista, *A Deterministic Projector Configuration Interaction Approach for the Ground State of Quantum Many-Body Systems.*, *J. Chem. Theory Comput.* 12, 4326 (2016).

[9] K. P. Hannon, C. Li, and F. A. Evangelista, *An integral-factorized implementation of the driven similarity renormalization group second-order multireference perturbation theory*, *J. Chem. Phys.* 144, 204111 (2016).

[10] J. B. Schriber and F. A. Evangelista, *Communication: An adaptive configuration interaction approach for strongly correlated electrons with tunable accuracy*, *J. Chem. Phys.* 144, 161106 (2016).

[11] C. Li and F. A. Evangelista, *Towards numerically robust multireference theories: The driven similarity renormalization group truncated to one- and two-body operators*, *J. Chem. Phys.* 144, 164114 (2016).

[12] P. Verma, W. D. Derricotte, and F. A. Evangelista, *Predicting Near Edge X-ray Absorption Spectra with the Spin-Free Exact-Two-Component Hamiltonian and Orthogonality Constrained Density Functional Theory.*, *J. Chem. Theory Comput.* 12, 144 (2016).

[13] C. Li and F. A. Evangelista, *Multireference Driven Similarity Renormalization Group: A Second-Order Perturbative Analysis*, *J. Chem. Theory Comput.* 11, 2097 (2015).

[14] W. D. Derricotte and F. A. Evangelista, *Simulation of X-ray absorption spectra with orthogonality constrained density functional theory*, *Phys. Chem. Chem. Phys.* 17, 14360 (2015).

[15] F. A. Evangelista, *A driven similarity renormalization group approach to quantum many-body problems*, *J. Chem. Phys.* 141, 054109 (2014).

[16] Z. Homayoon, J. M. Bowman, and F. A. Evangelista, *Calculations of Mode-Specific Tunneling of Double-Hydrogen Transfer in Porphycene Agree with and Illuminate Experiment*, *J. Phys. Chem. Lett.* 5, 2723 (2014).

[17] F. A. Evangelista, *Adaptive multiconfigurational wave functions*, *J. Chem. Phys.* 140, 124114 (2014).

[18] F. A. Evangelista, P. Shushkov, and J. C. Tully, *Orthogonality Constrained Density Functional Theory for Electronic Excited States*, *J. Phys. Chem. A* 117, 7378 (2013).

[19] F. A. Evangelista and J. Gauss, *On the approximation of the similarity-transformed Hamiltonian in single-reference and multireference coupled cluster theory*, *Chem. Phys.* 401, 27 (2012).

[20] J. I. Wu, Y. Mo, F. A. Evangelista, and P. v. R. Schleyer, *Is cyclobutadiene really highly destabilized by antiaromaticity?*, *Chem. Commun.* 48, 8437 (2012).

[21] F. A. Evangelista, M. Hanauer, A. Köhn, and J. Gauss, *A sequential transformation approach to the internally contracted multireference coupled cluster method*, *J. Chem. Phys.* 136, 204108 (2012).

[22] J. M. Turney, A. C. Simmonett, R. M. Parrish, et al., *Psi4: an open-source ab initio electronic structure program*, *WIREs Comput. Mol. Sci.* 2, 556 (2011).

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

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

[25] J. I. Wu, F. A. Evangelista, and P. v. R. Schleyer, *Why Are Perfluorocyclobutadiene and Some Other $(CF)_q^n$ Rings Non-Planar?*, *Org. Lett.* 12, 768 (2010).

[26] T. Lu, Q. Hao, A. C. Simmonett, et al., *Low-Lying Triplet States of Diphosphene and Diphosphinylidene*, *J. Phys. Chem. A* 114, 10850 (2010).

[27] 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).

[28] 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).

[29] 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).

[30] 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).

[31] 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).

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

[33] 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).

[34] 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).

[35] 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).

[36] 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).

[37] 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).

[38] 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).

[39] 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).

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

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

[42] 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).

Invited Conference Talks (since at Emory)

Feb. 2018	2018 Sanibel Symposium, Saint Simon Island, Georgia.
Aug. 2017	WATOC 2017, Munich, Germany.
Aug. 2017	254th ACS, Washington D.C.
Jul. 2017	ACTC 2017, Boston, Massachusetts.
Jun. 2017	TSRC: New Frontiers in Electron Correlation, Telluride, Colorado.
May 2017	SETCA 2017, University of Mississippi, Oxford, Mississippi.
Apr. 2017	253rd ACS, San Francisco, California.

Feb. 2017	Society of Industrial and Applied Mathematics 2017, Atlanta, Georgia.
Oct. 2016	ICT-HPCC16, Southwest University, Chongqing, China.
Jul. 2016	ISTCP-VI, Grand Forks, North Dakota.
Jun. 2016	TSRC: Low-scaling and Unconventional Electronic Structure Techniques, Telluride, Colorado.
May 2016	SETCA 2016, University of Tallahassee, Tallahassee, Florida.
Mar. 2016	251st ACS, San Diego, California.
Jul. 2015	TSRC: New Frontiers in Electron Correlation, Telluride, Colorado.
Jun. 2015	ICQC 2015, Satellite Symposium, Kobe University, Kobe, Japan.
Mar. 2015	249th ACS, Denver, Colorado.
Aug. 2014	248th ACS, San Francisco, California.
Jul. 2014	TSRC: Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride, Colorado.
Nov. 2013	SERMACS 2013, Atlanta, Georgia.
Sep. 2013	246th ACS, Indianapolis, Indiana.

Invited Lectures and Colloquia (since at Emory)

Oct. 2016	Physical Chemistry Seminar, University of California Irvine, Irvine, California.
Sept. 2016	Department Seminar, Auburn University, Auburn, Alabama.
Apr. 2016	Mathematics & Computer Science, Emory University, Atlanta, Georgia, USA.
Feb. 2016	Physical Chemistry Seminar, Rice University, Houston, Texas, USA.
Apr. 2015	Nuclear Physics, Michigan State University, East Lansing, Michigan.
Dec. 2013	ETH Zurich and IBM Zurich, Zurich, Switzerland.