CURRICULUM VITAE
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Chenyang Li

Contact Information

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Professional Experience

2021 — now	*Associate Professor*, Beijing Normal University, Beijing, China
2015 — 2020	*Postdoctoral Fellow*, Emory University, Atlanta, GA, USA Advisor: Professor Francesco A. Evangelista

Education

2012 — 2015	*Doctor of Philosophy*, University of Georgia, Athens, GA, USA Advisor: Professor Henry F. Schaefer III
2008 — 2012	*Bachelor of Science*, Nanjing University, Nanjing, Jiangsu, China Advisor: Professor Shuhua Li

Research Interests

- Developments of accurate electronic structure methods for excited states
- Developments of analytic energy gradients for low-order perturbation theories
- Theoretical studies of elementary hydrocarbon species in combustion chemistry
- Software developments

[1] Forte: an open-source plugin to Psi4 (https://github.com/psi4/psi4) that implements a variety of quantum chemistry methods for strongly correlated electrons. For the current version, see https://github.com/evangelistalab/forte.

[2] DSRG Generator: an automatic equation and code generator for second-quantized operators based on generalized normal ordering of Mukherjee and Kutzelnigg.

Teaching Experience

2013 summer	Lecturer for the quantum chemistry summer school Center for Computational Quantum Chemistry, The University of Georgia
2012 — 2013	Teaching assistant for General Chemistry Lab I and II Department of Chemistry, The University of Georgia

Publications

20. He, N.; **Li, C.** and Evangelista, F. A.* "Second-Order Active Space Embedding Theory" *J. Chem. Theory Comput. submitted*.
19. Wang, S.*; **Li, C.*** and Evangelista, F. A.* "Analytic Energy Gradients for the Driven Similarity Renormalization Group Multireference Second-Order Perturbation Theory" *J. Chem. Theory Comput. submitted*.
18. Huang, M.; **Li, C.** and Evangelista, F. A.* "Theoretical Calculation of Core-Excited States Along Dissociative Pathways Beyond Second-order Perturbation Theory" *J. Chem. Theory Comput. submitted*.

17. **Li, C.*** and Evangelista, F. A. "Spin-free implementation of the multireference driven similarity renormalization group: A benchmark study of open-shell diatomic molecules and spin-crossover energetics" *J. Chem. Phys.* **2021**, *155*, 114111.

16. Xu, Z.; Huang, Z.; **Li, C.***; Huang, T.; Evangelista, F. A.; Tang, M. L.* and Lian, T.* "Tuning the Quantum Dot (QD) / Mediator Interface for Optimal Efficiency of QD-Sensitized Near-Infrared-to-Visible Photon Upconversion Systems" *ACS Appl. Mater. Interfaces* **2020**, *12*, 36558–36567.

15. **Li, C.*** and Evangelista, F. A. "Connected Three-Body Terms in the Single-Reference Unitary Many-Body Theories: Iterative and Perturbative Approximations" *J. Chem. Phys.* **2020**, *152*, 234116.

14. Wang, S.; **Li, C.*** and Evangelista, F. A. "Analytic Gradients for Single-Reference Driven Similarity Renormalization Group Second-Order Perturbation Theory" *J. Chem. Phys.* **2019**, *151*, 044118. [Editor's Pick]

13. Zhang, T.*; **Li, C.*** and Evangelista, F. A.* "Towards Efficient Multireference Driven Similarity Renormalization Group Theory: Sequential Transformation Approach, Density Fitting and Non-Interacting Virtual Orbital Approximation" *J. Chem. Theory Comput.* **2019**, *15*, 4399–4414.

12. **Li, C.***; Lindh R.* and Evangelista, F. A.* "Dynamically-Weighted Multireference Perturbation Theory: Combining the Advantages of State-Specific and Multi-State Theories" *J. Chem. Phys.* **2019**, *150*, 144107.

11. **Li, C.*** and Evangelista, F. A.* "Multireference Theories of Electron Correlation Based on the Driven Similarity Renormalization Group" *Annu. Rev. Phys. Chem.* **2019**, *70*, 245–273.

10. Schriber, J. B.; Hannon, K. P.; **Li, C.** and Evangelista, F. A.* "A Combined Selected Configuration Interaction and Many-Body Treatment of Static and Dynamical Correlation in Oligoacenes" *J. Chem. Theory Comput.* **2018**, *14*, 6295–6305.

9. Huang, Y.; Xu, Z.; Jin, S.; **Li, C.**; Warncke, K.; Evangelista, F. A.*; Lian, T.* and Egap, E.* "Conjugated Oligomers with Stable Radical Substituents: Synthesis, Single Crystal Structures, Electronic Structure and Excited State Dynamics" *Chem. Mater.* **2018**, *30*, 7840–7851.

8. **Li, C.*** and Evangelista, F. A.* "Driven Similarity Renormalization Group for Excited States: A State-Averaged Perturbation Theory" *J. Chem. Phys.* **2018**, *148*, 124106. [Editor's Pick]

7. **Li, C.**; Verma, P.; Hannon, K. P. and Evangelista, F. A.* "A Low-Cost Approach to Electronic Excitation Energies Based on the Driven Similarity Renormalization Group" *J. Chem. Phys.* **2017**, *147*, 074107.

6. **Li, C.*** and Evangelista, F. A.* "Driven Similarity Renormalization Group: Third-Order Multireference Perturbation Theory" *J. Chem. Phys.* **2017**, *146*, 124132; Erratum: **2018**, *148*, 079902.

5. Hannon, K. P.; **Li, C.** and Evangelista, F. A.* "An Integral-Factorized Implementation of the Driven Similarity Renormalization Group Second-Order Multireference Perturbation Theory" *J. Chem. Phys.* **2016**, *144*, 204111.

4. **Li, C.** and Evangelista, F. A.* "Towards Numerically Robust Multireference Theories: The Driven Similarity Renormalization Group Truncated to One- and Two-Body Operators" *J. Chem. Phys.* **2016**, *144*, 164114; Erratum: **2018**, *148*, 079903.

3. **Li, C.** and Evangelista, F. A.* "Multireference Driven Similarity Renormalization Group: A Second-Order Perturbative Analysis" *J. Chem. Theory Comput.* **2015**, *11*, 2097–2108.

2. **Li, C.**; Agarwal, J.; Wu, C.-H.; Allen, W. D. and Schaefer, H. F.* "The Intricate Internal Rotation Surface and Fundamental Infrared Transitions of *n*-Propyl Radical" *J. Phys. Chem. B* **2015**, *119*, 728–735.

1. **Li, C.**; Agarwal, J. and Schaefer, H. F.* "The Remarkable $[ReH_9]^{2-}$ Dianion: Molecular Structure and Vibrational Frequencies" *J. Phys. Chem. B* **2014**, *118*, 6482–6490.

Oral Presentations

Apr. 2021 *32nd CCS Congress*, Zhuhai, Guangdong, China
Spin-Free Implementation of the Multireference Driven Similarity Renormalization Group

Jan. 2020 *Department of Chemistry, Beijing Institute of Technology*, Beijing, China
Connected Triples in the Single-Reference Unitary Many-Body Theories

Oct. 2019 (Withdraw) *Workshop on New Methods for Strongly Correlated Electrons*, Qingdao, China
Connected Triples in Single-Reference Driven Similarity Renormalization Group

Apr. 2019 *257th ACS National Meeting*, Orlando, FL, USA
Towards Perturbative Triples Corrections in the Multireference Driven Similarity Renormalization Group

Sept. 2018 *Atlanta Mini Symposium on Theoretical and Computational Chemistry*, Atlanta, GA, USA
Recent Developments of Multireference Driven Similarity Renormalization Group

May 2018 *Department of Physics, Northwest University*, Xi'an, Shaanxi, China
Recent Developments of Multireference Driven Similarity Renormalization Group

May 2018 *Chinese Academy of Sciences Computer Network Information Center*, Beijing, China
Recent Developments of Multireference Driven Similarity Renormalization Group

Poster Presentations

Oct. 2021 *14th National Conference of Quantum Chemistry (CCS)*, Shanghai, China
Analytic Energy Gradients for DSRG-MRPT2

July 2017 *American Conference on Theoretical Chemistry*, Boston, MA, USA
Driven Similarity Renormalization Group Multireference Perturbation Theory

May 2017 *Southeast Theoretical Chemistry Association*, Oxford, MS, USA
Driven Similarity Renormalization Group: Third-Order Multireference Perturbation Theory

July 2016 *International Society for Theoretical Chemical Physics*, Grand Forks, ND, USA
Driven Similarity Renormalization Group: Third-Order Multireference Perturbation Theory

Feb. 2016 *Sanibel Symposium*, St. Simons, GA, USA
Multireference Driven Similarity Renormalization Group Truncated to One- and Two-Body Operators

Oct. 2015 *Emerson Center Lectureship Award Symposium*, Atlanta, GA, USA
Multireference Driven Similarity Renormalization Group: A Second-Order Perturbative Analysis

May 2014 *Southeast Theoretical Chemistry Association*, Atlanta, GA, USA
The Intricate Internal Rotation Surface and Fundamental Infrared Transitions of *n*-Propyl Radical

Other Experience

[1] Algorithms, a four-course specialization by Stanford University on Coursera, earned on December 5, 2017

[2] Deep Learning, a five-course specialization by deeplearning.ai on Coursera (finished first four)

[3] Self-Driving Car Nano-Degree on Udacity (Term 1)

- Implemented a convolutional neural network (LeNet-5) to classify traffic signs using TensorFlow. [Link]
- Built a convolutional neural network using Keras that can autonomously drive a vehicle on the simulator. [Link]
- Implemented a pipeline to identify the lane boundaries in a video using OpenCV. [Link]