

## Curriculum Vitae

Stephen H. Yuwono, Graduate Assistant  
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## Education

2017 – present, pursuing Ph.D. in theoretical and computational chemistry at Michigan State University, U.S.A., Advisor: Professor Piotr Piecuch.

2016 – 2017, pursuing Ph.D. in theoretical and computational chemistry at Michigan State University, U.S.A., Advisor: Professor Angela K. Wilson.

2015 – 2016, pursuing Ph.D. in computational chemistry at the University of North Texas, U.S.A., Advisor: Professor Angela K. Wilson.

B.Sc. (Hons), 2015, Chemistry, National University of Singapore, Singapore.

## Professional Experience

Michigan State University, U.S.A., 2016 – present. Graduate Research Assistant and Teaching Assistant for freshman general chemistry and physical chemistry laboratory courses.

University of North Texas, U.S.A., 2015 – 2016. Teaching Assistant for a general chemistry class, computer laboratory, and physical and computational chemistry weekly sessions.

National University of Singapore, Singapore, 2014. Teaching Assistant for a freshman general chemistry laboratory.

## Research Experience

Michigan State University, 2017 – present, graduate research. I work on the development and applications of novel coupled-cluster (CC) methods and their extensions to excited states based on the equation-of-motion (EOM) CC formalism. This includes combining the deterministic  $CC(P;Q)$  and stochastic Quantum Monte Carlo (QMC) approaches to rapidly converge the high-level EOMCC (e.g., EOMCCSDT) energetics out of the early stages of QMC propagations. I have also investigated the rovibrational manifolds characterizing the ground and excited electronic states of the weakly bound magnesium dimer using the high-level CC and  $CC(P;Q)$  methods through quadruple excitations, the EOMCC methods through triple excitations, and the full configuration interaction approach. One of the consequences of this investigation has been an unprecedented *ab initio* simulation of the experimental laser-induced fluorescence spectra of the magnesium dimer

and its isotopologs that has allowed us to demonstrate the existence of a few additional vibrational levels of  $Mg_2$  that have eluded scientists for half a century. I have also been involved in a larger collaborative project aimed at the fundamental understanding of the behavior and properties of novel super photobases discovered at MSU designated as **FRO-SB**, which exhibits a change in  $pK_a$  by about 14 units upon photoexcitation. Advisor: Professor Piotr Piecuch.

University of North Texas / Michigan State University, 2015 – 2017, graduate research. As a follow-up of my earlier undergraduate research project in 2014, I benchmarked several DFT functionals in the geometry optimizations of lanthanide trihalides. I also evaluated the performance of various DFT methods in calculations of enthalpies of formation and bond dissociation energies of lanthanide-containing compounds. Advisor: Professor Angela K. Wilson.

National University of Singapore, 2014 – 2015, Honours Project in Chemistry. I conducted a mechanistic study of proline-tetrazole-catalyzed enantioselective N-nitroso aldol reaction of aldehydes. I investigated the system using a mechanism previously considered for another similar catalytic cycle. Advisor: Professor Ming Wah (Richard) Wong.

University of North Texas, 2014, International Research Experience for Undergraduates (IREU). I benchmarked several DFT functionals in the geometry optimizations of lanthanide trichlorides and tribromides. Advisor: Professor Angela K. Wilson.

National University of Singapore, 2013, Undergraduate Research Opportunities Programme in Science (UROPS). I studied the electron transfer through the scattering region in zigzag graphene nanoribbons, which are prototype systems for molecular-scale electronic junctions. Advisor: Professor Hway Chuan Kang.

## Awards

College of Natural Science Dissertation Completion Fellowship, Michigan State University, Spring 2022

2020 Longuet-Higgins Early Career Researcher Prize, awarded by the Editors of *Molecular Physics*, Taylor & Francis (Prize awarded in 2021)

College of Natural Science Dissertation Continuation Fellowship, Michigan State University, Summer 2020

Education Merit Award for Excellence in Teaching, Michigan State University, Spring 2018

Education Merit Award for Excellence in Teaching, Michigan State University, Fall 2017

Tertiary education scholarship from the Indonesian Ministry of Education for the medalists of International Science Olympiads, 2011 – 2015

Gold medal, International Chemistry Olympiad in Ankara, Turkey, 2011

Bronze medal, International Chemistry Olympiad in Tokyo, Japan, 2010

## Publications

1. L.E. Aebersold, S.H. Yuwono, G. Schoendorff, and A.K. Wilson, “Efficacy of Density Functionals and Relativistic Effective Core Potentials for Lanthanide-Containing Species: The Ln54 Molecule Set”, *J. Chem. Theory Comput.* **13**, 2831-2839 (2017).
2. S.H. Yuwono, I. Magoulas, J. Shen, and P. Piecuch, “Application of the Coupled-Cluster CC( $P;Q$ ) Approaches to the Magnesium Dimer”, *Mol. Phys.* **117**, 1486-1506 (2019) [Special Memorial Issue in Honour of Professor Dieter Cremer; invited contribution, in response to an invitation issued to P. Piecuch].
3. J.E. Deustua, S.H. Yuwono, J. Shen, and P. Piecuch, “Communication: Accurate Excited-State Energetics by a Combination of Monte Carlo Sampling and Equation-of-Motion Coupled-Cluster Computations”, *J. Chem. Phys.* **150**, 111101-1 – 111101-7 (2019).
4. J. Lahiri, M. Moemeni, J. Kline, B. Borhan, I. Magoulas, S.H. Yuwono, P. Piecuch, J.E. Jackson, M. Dantus, and G.J. Blanchard, “Proton Abstraction Mediates Interactions between the Super Photobase FR0-SB and Surrounding Alcohol Solvent”, *J. Phys. Chem. B* **123**, 8448-8456 (2019).
5. S.H. Yuwono, I. Magoulas, and P. Piecuch, “Quantum Computation Solves a Half-Century-Old Enigma: Elusive Vibrational States of Magnesium Dimer Found”, *Sci. Adv.*, **6**, eaay4058 (2020) (12 pages).
6. J. Lahiri, M. Moemeni, I. Magoulas, S.H. Yuwono, J. Kline, B. Borhan, P. Piecuch, J.E. Jackson, G.J. Blanchard, and M. Dantus, “Steric Effects in Light-Induced Solvent Proton Abstraction”, *Phys. Chem. Chem. Phys.*, **22**, 19613-19622 (2020).
7. S.H. Yuwono, A. Chakraborty, J.E. Deustua, J. Shen, and P. Piecuch, “Accelerating Convergence of Equation-of-Motion Coupled-Cluster Computations Using the Semi-Stochastic CC( $P;Q$ ) Formalism”, *Mol. Phys.*, **118**, e1817592 (2020) (17 pages) [Special Issue in Honour of Professor Jürgen Gauss; invited contribution, in response to an invitation issued to P. Piecuch].
8. J. Lahiri, M. Moemeni, J. Kline, I. Magoulas, S.H. Yuwono, M. Laboe, J. Shen, B. Borhan, P. Piecuch, J.E. Jackson, G.J. Blanchard, and M. Dantus, “Isoenergetic Two-Photon Excitation Enhances Solvent-to-Solute Excited-State Proton Transfer”, *J. Chem. Phys.*, **153**, 224301-1 – 224301-14 (2020); [arXiv:2010.04323](https://arxiv.org/abs/2010.04323).
9. J. Lahiri, S.H. Yuwono, I. Magoulas, M. Moemeni, B. Borhan, G.J. Blanchard, P. Piecuch, and M. Dantus, “Spectral Phase Control of the Quantum Interference between Two-Photon Optical Excitation Pathways”, *J. Phys. Chem. A*, **125**, 7534-7544 (2021); [arXiv:2103.09912](https://arxiv.org/abs/2103.09912).
10. B.A. Capistran, S.H. Yuwono, M. Moemeni, S. Maity, A. Vahdani, B. Borhan, J.E. Jackson, P. Piecuch, M. Dantus, and G.J. Blanchard, “Excited State Dynamics of a Substituted Fluorene Derivative. The Central Role of Hydrogen Bonding Interactions with the Solvent”, *J. Phys. Chem. B*, **125**, 12242-12253 (2021).

11. B.A. Capistran, S.H. Yuwono, M. Moemeni, S. Maity, A. Vahdani, B. Borhan, J.E. Jackson, P. Piecuch, M. Dantus, and G.J. Blanchard, “Intramolecular Relaxation Dynamics Mediated by Solvent-Solute Interactions of Substituted Fluorene Derivatives. Solute Structural-Dependence”, *J. Phys. Chem. B*, **125**, 12486-12499 (2021).
12. A. Chakraborty, S.H. Yuwono, J.E. Deustua, J. Shen, and P. Piecuch, “Benchmarking the Semi-Stochastic CC( $P;Q$ ) Approach for Singlet–Triplet Gaps in Biradicals”, manuscript in preparation.

### Poster Presentations Given by Stephen H. Yuwono

1. S.H. Yuwono, R. Weber, G. Schoendorff, A.K. Wilson, “Assessment of the Structural Prediction of Lanthanide Species Using DFT”, 26th Austin Symposium on Molecular Structure and Dynamics, Dallas, Texas, U.S.A., March 5-7, 2016.
2. S.H. Yuwono, R. Weber, G. Schoendorff, A.K. Wilson, “Comparison of DFT Functionals for the Structural Prediction of Lanthanide Species”, 251st American Chemical Society National Meeting, San Diego, California, U.S.A., March 13-17, 2016.
3. S.H. Yuwono, R. Weber, G. Schoendorff, A.K. Wilson, “Structural Optimization of Lanthanide Trihalides via Density Functional Theory”, Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.
4. S.H. Yuwono, I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, “Application of the CC( $P;Q$ ) Hierarchy of Coupled-Cluster Methods to the Challenging Beryllium and Magnesium Dimers”, 50th Midwest Theoretical Chemistry Conference, University of Chicago, Chicago, Illinois, U.S.A., June 21-23, 2018.

### Talks and Posters Presented by Co-Authors

1. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, “Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” TSRC Workshop “New Frontiers in Electron Correlation,” 2nd edition, Telluride, Colorado, U.S.A., June 10-14, 2019 [invited talk given by P. Piecuch].
2. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, “Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” Tenth Congress of the International Society for Theoretical Chemical Physics (ISTCP-X), symposium entitled “Emergent Electronic Structure Methods,” Tromsø, Norway, July 11-17, 2019 [invited talk given by P. Piecuch].
3. J.E. Deustua, I. Magoulas, S.H. Yuwono, J. Shen, and P. Piecuch, “Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster and Equation-of-Motion Coupled-Cluster Computations,” Tenth Congress of the International

Society for Theoretical Chemical Physics (ISTCP-X), Tromsø, Norway, July 11-17, 2019 [poster presented by J.E. Deustua].

4. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, “Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” 8th Conference “Current Trends in Theoretical Chemistry” (CTTC VIII), Cracow, Poland, September 1-4, 2019 [invited talk given by P. Piecuch].
5. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, and S.H. Yuwono, “Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” 20th International Conference on Recent Progress in Many-Body Theories, Toulouse, France, September 9-13, 2019 [invited talk given by P. Piecuch].
6. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, “Toward Exact Quantum Chemistry by a Combination of Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” The Utah Workshop on Quantum Methods in Molecular and Solid-State Theory, Park City, Utah, U.S.A., September 22-27, 2019 [invited talk given by P. Piecuch].
7. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, “Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” Workshop on New Methods for Strongly Correlated Electrons, Qingdao, China, October 9-13, 2019 [invited talk given by P. Piecuch].
8. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, “Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” The international conference “Quantum International Frontiers 2019,” Shanghai, China, November 18-22, 2019 [invited Frontier Lecture given by P. Piecuch].
9. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, and A. Chakraborty, “Approaching Exact Quantum Chemistry by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations,” the 60th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 16-21, 2020 [invited talk given by P. Piecuch].
10. P. Piecuch, J.E. Deustua, J. Shen, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, “High-Accuracy Electronic Energetics by Stochastic and Deterministic Wave Function Sampling and Coupled-Cluster Computations,” TSRC Workshop “Low-Scaling and Unconventional Electronic Structure Techniques” (LUEST 2020), 5th edition, Telluride, Colorado, U.S.A., June 1-5, 2020. **DUE TO COVID-19, REPLACED BY VIRTUAL WORKSHOP, June 1-5 and June 8-9, 2020** [invited talk given by P. Piecuch via Zoom].
11. P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, “Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations,” TSRC Workshop “New Frontiers in Electron Correlation,” 3rd edition, Telluride, Colorado, U.S.A., June 14-18, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].

12. P. Piecuch, J. Shen, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, and K. Gururangan, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," TSRC Workshop "New Developments in Coupled-Cluster Theory," Telluride, Colorado, U.S.A., July 19-23, 2021 [hybrid format; invited talk given by P. Piecuch via Zoom].
13. J. Lahiri, M. Moemeni, J. Kline, S.H. Yuwono, I. Magoulas, M. Laboe, J. Shen, B. Borhan, P. Piecuch, J.E. Jackson, and G.J. Blanchard, and M. Dantus, "Proton Abstraction Mechanism of the "Super" Photobase FR0-SB," 262nd American Chemical Society National Meeting, Atlanta, Georgia, U.S.A., August 22-26, 2021. [hybrid format; poster presented by J. Lahiri].
14. P. Piecuch, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations" (with contributions from J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen), International Symposium on Correlated Electrons (SymCorrel21), Munich Center for Quantum Science and Technology, Munich, Germany, October 5-7, 2021 [virtual workshop; invited talk given by P. Piecuch via Zoom].
15. P. Piecuch, S.H. Yuwono, I. Magoulas, and J. Shen, "Computational Studies of FR0-SB, a Novel Organic Compound that Deprotonates Alcohols Upon Photoexcitation," International conference in the series "New Horizons in Scientific Software (NHSS 2021)" entitled "Light-Matter Interaction: Theory Meets Experiment," Jeju Island, South Korea, November 22-25, 2021 [hybrid format; invited talk given jointly by P. Piecuch and S.H. Yuwono via Zoom].
16. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," The Seventeenth Theoretical Chemistry Symposium (TCS 2021), Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia, West Bengal, India, December 11-14, 2021 [virtual symposium; invited plenary lecture given by P. Piecuch].
17. M. Dantus, J. Lahiri, M. Moemeni, J. Kline, B. Borhan, I. Magoulas, S.H. Yuwono, P. Piecuch, J.E. Jackson, and G.J. Blanchard, "Design Dynamics and Quantum Theory of Reversible Super Photobases," The symposium "Frontiers in Ultrafast Spectroscopy of Photoexcited States," the 2020 International Chemical Congress of Pacific Basin Societies (Pacifichem 2020), Honolulu, Hawaii, U.S.A., December 15-20, 2020 [invited talk given by M. Dantus]. **DUE TO COVID-19, RESCHEDULED TO December 16-21, 2021 as hybrid congress.**
18. P. Piecuch, J.E. Deustua, I. Magoulas, S.H. Yuwono, A. Chakraborty, K. Gururangan, and J. Shen, "Approaching Exact Quantum Chemistry by Semi-Stochastic and Selected-CI-Driven Coupled-Cluster Computations," Chris Cramer 60th Birthday Symposium, 263rd American Chemical Society National Meeting, San Diego, California, U.S.A., March 20-24, 2022 [hybrid symposium; pre-recorded virtual presentation; invited talk given by P. Piecuch].