

Curriculum Vitae

Ilias Magoulas, Graduate Assistant
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Education

August 2015 – present, pursuing Ph.D. in theoretical and computational chemistry at Michigan State University, U.S.A., Advisor: Professor Piotr Piecuch.

M.S., 2013, Physical Chemistry, National and Kapodistrian University of Athens, Greece, Advisor: Assistant Professor Apostolos Kalamos.

B.S., 2011, Chemistry, National and Kapodistrian University of Athens, Greece, Undergraduate Thesis Advisor: Professor Aristides Mavridis.

Professional Experience

Michigan State University, U.S.A., August 2015 – present, Graduate Teaching and Research Assistant. Teaching senior level quantum chemistry courses while performing Ph.D. research in theoretical and computational chemistry. Ph.D. Advisor: Professor Piotr Piecuch.

Hellenic Army Chemistry Laboratory, Greece, August 2014 – March 2015, Assistant Analyst at the Textile Laboratory.

National and Kapodistrian University of Athens, Greece, July 2013 – June 2014, Voluntary Researcher in Professor Aristides Mavridis' Group.

National and Kapodistrian University of Athens, Greece, August 2011 – June 2013, Graduate Teaching and Research Assistant. I was a laboratory instructor for the laboratory of Physical Chemistry while performing M.S. research in theoretical and computational chemistry. M.S. Advisor: Assistant Professor Apostolos Kalamos.

Research Experience

Michigan State University, U.S.A., August 2015 – present, Graduate Student Researcher, Advisor: Professor Piotr Piecuch. I am currently working on the development and applications of novel coupled-cluster (CC) methods for strongly correlated systems. In the meantime, I worked on approaching exact full configuration interaction (FCI) energetics, at the computational cost of CC with singles and doubles, by cluster analysis of FCI quantum Monte Carlo wave functions. This

investigation resulted in one publication in the *Journal of Chemical Physics*. I have also explored the ability of the CC(*P;Q*) hierarchy of CC methods to accurately reproduce the CCSDT and CCSDTQ potential energy curves and spectroscopic data of challenging weakly bound diatomics, including the Be₂ and Mg₂ dimers. This work resulted in two publications, one in the *Journal of Physical Chemistry A* for Be₂ and the other in *Molecular Physics* for the case of Mg₂. Representative results have been presented in talks and a couple of posters. My work has also included a collaboration between our group and the group of professor Dantus, where we examined the predissociation of sodium iodide in the A 0⁺ state. For this project I constructed the potential energy curves of thirteen spin-orbit-coupled states of sodium iodide using multi-reference configuration interaction (MRCI). In addition, I calculated the vibrational energies and wavefunctions for all vibrational levels of the X and A 0⁺ states. This study resulted in a publication in *Chemical Physics Letters*.

National and Kapodistrian University of Athens, Greece, July 2013 – June 2014, Voluntary Researcher in Professor Aristides Mavridis' group. I performed CC and MRCI calculations on temporary anions, testing the limitations of stationary methods. This work resulted in a publication in the *International Journal of Quantum Chemistry*. In addition, I studied through CC methods the van der Waals diatomic systems BNg in their ground and first excited state, and the corresponding C_{2v}-symmetric triatomics, BNg₂, in their ground electronic state, where Ng is a noble gas from He through Xe. This work resulted in a publication in the *Journal of Physical Chemistry A*.

National and Kapodistrian University of Athens, Greece, August 2011 – June 2013, Graduate Student Researcher, Advisor: Assistant Professor Apostolos Kalemos. My research was focused on the elucidation of the chemical bond in diatomic species using CC and MRCI methods. The systems studied were BF, BF⁺, BAs, BO, BO⁺, and BO⁻. This research resulted in three publications in the *Journal of Chemical Physics*.

Awards

49th Midwest Theoretical Chemistry Conference, East Lansing, MI, 2017: My collaborator, Jialin Liu, and I won one of the Journal of Physical Chemistry Best Student Poster awards.

Michigan State University, U.S.A., Spring Semester 2017: Education Merit Award for Excellence in Teaching.

National and Kapodistrian University of Athens, Greece, Academic Year 2009 – 2010: Hellenic State Scholarships Foundation honorific scholarship and award for outstanding academic performance.

National and Kapodistrian University of Athens, Greece, Academic Year 2007 – 2008: Hellenic State Scholarships Foundation honorific scholarship and award for outstanding academic performance.

Publications

- 1) Magoulas, A. Kalemos, and A. Mavridis, "An *ab Initio* Study of the Electronic Structure of

- BF and BF⁺”, *J. Chem. Phys.* **138**, 104312-1 – 104312-12 (2013).
- 2) Magoulas, and A. Kalemou, “An *ab Initio* Study of the Electronic Structure of Boron Arsenide, BAs”, *J. Chem. Phys.* **139**, 154309-1 – 154309-11 (2013).
 - 3) I. Magoulas, A. Papakondylis, and A. Mavridis, “Accurate *ab Initio* Structural Parameters of the Diatomic and Triatomic van der Waals Molecules ¹¹BNg (X²Π, A²Σ⁺) and ¹¹BNg₂ (X̃B₁), Ng = ⁴He, ²⁰Ne, ⁴⁰Ar, ⁸⁴Kr, and ¹³²Xe”, *J. Phys. Chem. A* **118**, 3990 – 3995 (2014).
 - 4) I. Magoulas, and A. Kalemou, “An *ab Initio* Study of the Electronic Structure of the Boron Oxide Neutral (BO), Cationic (BO⁺), and Anionic (BO⁻) Species”, *J. Chem. Phys.* **141**, 124308-1 – 124308-10 (2014).
 - 5) I. Magoulas, A. Papakondylis, and A. Mavridis, “Structural Parameters of the Ground States of the Quasi-Stable Diatomic Anions CO⁻, BF⁻, and BCl⁻ as Obtained by Conventional *ab Initio* Methods”, *Int. J. Quantum Chem.* **115**, 771 – 778 (2015).
 - 6) G. Rasskazov, M. Nairat, I. Magoulas, V.V. Lozovoy, P. Piecuch, and M. Dantus, “Femtosecond Real-Time Probing of Reactions MMXVII: The Predissociation of Sodium Iodide in the A 0⁺ State”, *Chem. Phys. Lett.* **683**, 121 – 127 (2017) [the Zewail Memorial Issue; invited contribution, in response to an invitation issued to M. Dantus].
 - 7) I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, “Application of the CC(*P*;*Q*) Hierarchy of Coupled-Cluster Methods to the Be₂ Dimer”, *J. Phys. Chem. A* **122**, 1350 – 1368 (2018) [special issue in honor of Professors Manuel Yáñez and Otilia Mó; invited contribution, in response to an invitation issued to P. Piecuch].
 - 8) J.E. Deustua, I. Magoulas, J. Shen, and P. Piecuch, “Communication: Approaching Exact Quantum Chemistry by Cluster Analysis of Full Configuration Interaction Quantum Monte Carlo Wave Functions”, *J. Chem. Phys.* **149**, 151101-1 – 151101-6 (2018).
 - 9) 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.*, in press [special memorial issue in honor of Professor Dieter Cremer; invited contribution, in response to an invitation issued to P. Piecuch].
 - 10) S.H. Yuwono, I. Magoulas, and P. Piecuch, “Resolving a Half-Century-Old Enigma: The Elusive *v*" = 14–18 Vibrational Levels of Mg₂”, manuscript in preparation.

Poster Presentations Given by Ilias Magoulas

- 1) I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, “Application of the CC(*P*;*Q*) Hierarchy of Coupled-Cluster Methods to the Challenging Problem of Be₂”, Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016.
- 2) J. Liu, I. Magoulas, Y. Qi, and P. Piecuch, “Cluster Approach for Predicting the Open Circuit Voltage in Energy Storage Materials Using High-Accuracy Quantum Chemistry Calculations”, 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presented by J. Liu and I. Magoulas].
- 3) I. Magoulas, J. Shen, and P. Piecuch, “Coupled-Cluster Approaches for Strongly Correlated

Systems”, 50th Midwest Theoretical Chemistry Conference, The University of Chicago, Chicago, Illinois, U.S.A, June 21-23, 2018.

Talks and Posters Presented by Co-Authors

- 1) P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, “Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems”, TSRC Workshop “Low-Scaling and Unconventional Electronic Structure Techniques” (LUEST 2016), 3rd edition, Telluride, Colorado, U.S.A., June 1-5, 2016 [invited talk given by P. Piecuch].
- 2) P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, “Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: $CC(P;Q)$ Formalism”, Ninth Congress of the International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, North Dakota, U.S.A., July 17-22, 2016 [invited talk given by P. Piecuch].
- 3) P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, “Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: $CC(P;Q)$ Formalism”, The International Conference “Theory and Applications of Computational Chemistry 2016 (TACC 2016)”, Seattle, Washington, August 28 – September 2, 2016 [invited talk given by P. Piecuch].
- 4) J. Shen, N.P. Bauman, I. Magoulas, and P. Piecuch, “Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: $CC(P;Q)$ Formalism”, 49th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 1-3, 2017 [poster presented by J. Shen].
- 5) P. Piecuch, J. Shen, N.P. Bauman, and I. Magoulas, “Single-Reference Coupled-Cluster and Equation-of-Motion Coupled-Cluster Methods for Multi-Reference Problems: $CC(P;Q)$ Formalism”, The symposium “Electronic Structure of Complex Chemical Systems”, 254th American Chemical Society National Meeting, Washington, DC, U.S.A., August 20-24, 2017 [invited talk given by P. Piecuch].
- 6) 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, The University of Chicago, Chicago, Illinois, U.S.A, June 21-23, 2018. [poster presented by S.H. Yuwono].
- 7) P. Piecuch, J.E. Deustua, J. Shen, and I. Magoulas, “Toward Exact Quantum Chemistry: Accurate Electronic Energies by Stochastic Wave Function Sampling and Deterministic Coupled-Cluster Computations”, The international conference “Quantum International Frontiers 2018”, Changsha, Hunan Province, China, October 17-21, 2018 [invited Frontier Lecture given by P. Piecuch].