Anh H. Reynolds

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Education and Work Experience

Chemistry Teacher **2018–2019**
Miami Country Day School, Miami, FL

MS in Theoretical Chemistry **2013–2018**
Northwestern University, Evanston, IL *Advisor: Prof. Toru Shiozaki*

- Developed and implemented an efficient algorithm that scales well in parallel to compute the exchange integrals—bottleneck in quantum mechanical calculations
- Part of the team developing and maintaining BAGEL, a C++ electronic structure library under the GNU General Public License (nubakery.org)

Research Scholar **2012–2013**
Université Paul Sabatier, Toulouse, France *Advisor: Prof. Stefano Evangelisti*

- Studied the electronic and structure properties of cyclacenes—building blocks of single-walled carbon nanotubes, using multi-reference methods.

Research Assistant **2010–2012**
National University of Singapore, Singapore *Advisor: Prof. Ryan Bettens*

- Developed and implemented an energy-based fragmentation method in Fortran to study large complex molecular systems.

Visiting Research Scholar **2009**
Australian National University, Canberra, Australia *Advisor: Prof. Michael Collins*

- Constructed an interpolated multidimensional surface to simulate the reaction dynamics of H_3^+ and CO, abundant species in insterstellar environments.

BS in Chemistry (1st Class Honors) **2006–2010**
National University of Singapore, Singapore

Skills

- C++, Python, Octave, Fortran, Linux Command Line, Bash Shell Scripting
- Pandas, NumPy, SciPy, scikit-learn, TensorFlow, Keras
- Latex, gnuplot, matplotlib, Adobe Illustrator
- Machine learning algorithms: regression, classification, neural networks

Coursera Certifications

Machine Learning, *Stanford University*
Deep Learning Specialization (5 courses), *deeplearning.ai*
Applied Text Mining in Python, *University of Michigan*
Applied Machine Learning in Python, *University of Michigan*
Introduction to Data Science in Python, *Univeristy of Michigan*
Mathematical Biostatistics Bootcamp I, *John Hopkins University*

Publications

Hai-Anh Le and Toru Shiozaki, Occupied-orbital fast multipole method for efficient exact exchange evaluation, *J. Chem. Theory Comput*, **2018**, *14*, 1228–1234.

Stefano Battaglia, Hai-Anh Le, Gian L. Bendazzoli, Noelia Faginas-Lago, Thierry Leininger, and Stefano Evangelisti, A theoretical study on cyclacenes: Analytical tight-binding approach, *Int. J. Quantum Chem.*, **2018**, *118*, e25569.

Hai-Anh Le, Hwee-Jia Tan, John F. Ouyang, and Ryan P. A. Bettens, Combined Fragmentation Method: A Simple Method for Fragmentation of Large Molecules, *J. Chem. Theory Comput*, **2012** *8*, 469–478.

Hai-Anh Le and Ryan P. A. Bettens, Distributed Multipoles and Energies of Flexible Molecules, *J. Chem. Theory Comput*, **2011**, *7*, 921–930.

Hai-Anh Le, Terry J. Frankcombe, and Michael A. Collins, Reaction Dynamics of H_3^+ + CO on an Interpolated Potential Energy Surface, *J. Phys. Chem. A*, **2010**, *114*, 10783–10788.

Hai-Anh Le, Adrian M. Lee, and Ryan P. A. Bettens, Accurately Reproducing Ab Initio Electrostatic Potentials with Multipoles and Fragmentation, *J. Phys. Chem. A*, **2009**, *113*, 10527–10533.

Conferences

49th Midwest Theoretical Chemistry Conference (Poster) *East Lansing, MI*	2017
Theory and Applications of Computational Chemistry (Poster) *Seattle, WA*	2016
48th Midwest Theoretical Chemistry Conference(Poster) *Pittsburgh PA*	2016
47th Midwest Theoretical Chemistry Conference (Poster) *Ann Arbor, MI*	2015
Theoretical Chemistry for Periodic Systems (Oral) *Ax-les-Thermes, France*	2013
AIQC: Interfacing Electronic Structure with Dynamics (Poster) *Minneapolis, MN*	2012
International Conference on Computational Science and Engineering (Oral) *Ho Chi Minh City, Vietnam*	2011
9th Triennial Congress of the WATOC (Poster) *Santiago de Compostela, Spain*	2011
National Undergraduate Research Opportunities Programme Congress (Oral) *Singapore, Singapore*	2010
National Undergraduate Research Opportunities Programme Congress (Oral) *Singapore, Singapore*	2009

Honours and Awards

Poster Award, 49th Midwest Theoretical Chemistry Conference	2017
Poster Award, 47th Midwest Theoretical Chemistry Conference	2015
Burwell Summer Scholarship	2015
Erasmus Mundus Scholarship	2012–2013
President Graduate Fellowship	2010
ASEAN Undergraduate Scholarship	2006–2010
CRISP Award for the best undergraduate research project	2010
Schering-Plough Gold Medal for the best under graduate research project	2009