

Anh H. Reynolds

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SUMMARY

- Highly motivated with strong scientific research and programming background
- Excellent at communicating technical concepts to a wide range of audience
- Experienced in C++, Python, and shell scripting
- Familiar with machine learning literature and optimization techniques
- Graduate research focused on electronic structure theory, making quantum chemistry accessible to large-scale problems through an open-source program written in C++, BAGEL (nubakery.org).

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

Machine Learning, *Stanford University*

CERTIFICATIONS

Applied Text Mining in Python, *University of Michigan*

Applied Machine Learning in Python, *University of Michigan*

Introduction to Data Science in Python, *University of Michigan*

Deep Learning Specialization (5 courses), *deeplearning.ai*

EDUCATION AND WORK

AP Chemistry Teacher

2018–2019

Miami Country Day School, Miami, FL

EXPERIENCE

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 Toulouse III - Paul Sabatier, Toulouse, France

- 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

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

BS in Chemistry (1st Class Honors)

2006–2010

National University of Singapore, Singapore

PUBLICATIONS	<u>Hai-Anh Le</u> and Toru Shiozaki, Occupied-orbital fast multipole method for efficient exact exchange evaluation, <i>J. Chem. Theory Comput</i> , 2018 , 14, 12281234.	
	Stefano Battaglia, <u>Hai-Anh Le</u> , Gian L. Bendazzoli, Noelia Faginas-Lago, Thierry Leininger, and Stefano Evangelisti, A theoretical study on cyclacenes: Analytical tight-binding approach, <i>Int. J. Quantum Chem.</i> , 2018 , 118, e25569.	
	<u>Hai-Anh Le</u> , Hwee-Jia Tan, John F. Ouyang, and Ryan P. A. Bettens, Combined Fragmentation Method: A Simple Method for Fragmentation of Large Molecules, <i>J. Chem. Theory Comput</i> , 2012 8, 469–478.	
	<u>Hai-Anh Le</u> and Ryan P. A. Bettens, Distributed Multipoles and Energies of Flexible Molecules, <i>J. Chem. Theory Comput</i> , 2011 , 7, 921–930.	
	<u>Hai-Anh Le</u> , Terry J. Frankcombe, and Michael A. Collins, Reaction Dynamics of $H_3^+ + CO$ on an Interpolated Potential Energy Surface, <i>J. Phys. Chem. A</i> , 2010 , 114, 10783–10788.	
	<u>Hai-Anh Le</u> , Adrian M. Lee, and Ryan P. A. Bettens, Accurately Reproducing Ab Initio Electrostatic Potentials with Multipoles and Fragmentation, <i>J. Phys. Chem. A</i> , 2009 , 113, 10527–10533.	
CONFERENCES	49th Midwest Theoretical Chemistry Conference (Poster)	2017
	<i>East Lansing, MI</i>	
	Theory and Applications of Computational Chemistry (Poster)	2016
	<i>Seattle, WA</i>	
	48th Midwest Theoretical Chemistry Conference (Poster)	2016
	<i>Pittsburgh PA</i>	
	47th Midwest Theoretical Chemistry Conference (Poster)	2015
	<i>Ann Arbor, MI</i>	
	Theoretical Chemistry for Periodic Systems (Oral)	2013
	<i>Ax-les-Thermes, France</i>	
HONOURS AND AWARDS	AIQC: Interfacing Electronic Structure with Dynamics (Poster)	2012
	<i>Minneapolis, MN</i>	
	International Conference on Computational Science and Engineering (Oral)	2011
	<i>Ho Chi Minh City, Vietnam</i>	
	9th Triennial Congress of the WATOC (Poster)	2011
	<i>Santiago de Compostela, Spain</i>	
	National Undergraduate Research Opportunities Programme Congress (Oral)	2010
	<i>Singapore, Singapore</i>	
	National Undergraduate Research Opportunities Programme Congress (Oral)	2009
	<i>Singapore, Singapore</i>	
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 (declined)	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