

PRAJAY PATEL

Argonne National Laboratory | Chemical Sciences and Engineering Division

9700 S. Cass Ave Building 241 Room A265A, Lemont, IL, 60439

Email: patelp@anl.gov

Phone: (+1) 630-252-7706

Website: <https://www.linkedin.com/in/prajay-patel/>

Nationality: US-Canadian Dual Citizen

EDUCATION

Ph.D. in Physical Chemistry, Michigan State University (MSU) August 2014 - August 2019

Moved to MSU with research advisor from University of North Texas (UNT)

Advisor: Angela K. Wilson; GPA 3.95/4.00

B.S. in Chemistry and Mathematics, University of Texas at Arlington (UTA) August 2010 - May 2014

Summa Cum Laude, GPA: 3.92/4.00

PROFESSIONAL EXPERIENCE

Postdoctoral Appointee August 2019 - Present

Chemical Sciences and Engineering Division, Argonne National Laboratory

- Mentors: Cong Liu and Massimiliano Delferro
- Topics: X-ray absorption spectroscopy (XANES), computational catalysis, transition metals, machine learning

Graduate Research Assistant October 2014 - July 2019

Department of Chemistry, UNT and MSU

- Advisor: Angela K. Wilson
- Topics: Local correlation, potential energy surfaces, transition metals, high accuracy thermochemistry, catalysis

Graduate Teaching Assistant August 2014 - May 2017

Department of Chemistry, UNT and MSU

- General and Physical Chemistry Labs and Lectures

Computational Chemistry Instructional Laboratory Assistant May 2015 - May 2016

Department of Chemistry, UNT

Chemistry Clinic Tutor June 2013 - May 2014

Department of Chemistry and Biochemistry, UTA

Undergraduate Research Assistant June 2012 - May 2014

Department of Chemistry and Biochemistry, UTA

- Advisor: Peter Kroll
- Topic: Computational materials

Math Clinic Tutor January 2012 - May 2014
Department of Mathematics, UTA

- Served as the exclusive statistics tutor for undergraduate and graduate students from 2013 to 2014
- **Received tutor of the year for 2014**

Bio-engineering Project Mentor and Residential Facilitator June 2012 - August 2012
College of Engineering, UTA

- Worked with 7th-10th grade students during the Engineering and Computer Science Summer Camps

Mathematics Project Mentor and Industrial Engineering Project Mentor August 2011
College of Engineering, UTA

- Worked with high school students who placed in the Texas state science fair

Electrical Engineering Project Mentor June 2011 - August 2011
College of Engineering, UTA

- Worked with Grade 5-10 students during the Engineering and Computer Science Summer Camps

MENTORING EXPERIENCE

Graduate Student: Woochul Shin (ANL)	2019
Research Experience for Undergraduates: Betoul Ali (MSU)	2019
RISE Worldwide from German Academic Exchange Service: Rebecca Tomann (MSU)	2019
High School Student: Joseph Chung (MSU)	2018-2019
High School Honors Science, Math, and Engineering Program: Max Bowman (MSU)	2018-2019
Undergraduate Research Assistant through Honors College: Sam Ryan (MSU)	2017-2019
Welch Summer Scholar Program: Miki Somosot (UTA)	2013

PROFESSIONAL MEMBERSHIPS

National Postdoctoral Association	2019-Present
Michigan Catalysis Society / Michigan Chapter of the North American Catalysis Society	2017-Present
American Chemical Society Younger Chemists Committee	2016-2019
American Chemical Society (ACS)	2013-Present
Mathematical Association of America	2013-2014
Phi Kappa Phi National Honor Society	2012-2013
National Society of Leadership and Success	2011

AWARDS

College of Natural Science Dissertation Continuation Fellowship (MSU)	2019
College of Arts and Sciences Graduate Student Support Grant Recipient (UNT)	2015-2016
Graduate Assistantship Tuition Scholarship (UNT)	2014-2015
Math Clinic Tutor of the Year (UTA)	2014
Mathematics Outstanding Senior (UTA)	2014
H.A.D. Dunsworth Scholarship (UTA)	2013-2014
Daniel and Linda Armstrong Scholarship (UTA)	2013-2014
College of Science Dean's List for Academic Excellence (UTA)	2012-2014
National Science Foundation Robert Noyce Summer Internship Recipient	2011
Academic Enhancement Scholarship (UTA)	2011-2014
President's Charter Scholarship (UTA)	2010-2014

Coordinating Board Top 10 Percent Scholarship (UTA)
Top 10 Percent Scholarship (UTA)

2010-2014
2010-2014

PUBLICATIONS

1. Patel, P.; Kuntz, D. M.; Jones, M. R.; Wilson, A. K. SAMPL6 LogP Challenge: Machine Learning and Quantum Mechanical Approaches *J. Comput. Aided. Mol. Des.* **2020**, <https://doi.org/10.1007/s10822-020-00287-0>.
2. Patel, P. and Wilson, A. K. Domain-based Local Pair Natural Orbital Methods within the Correlation Consistent Composite Approach. *J. Comput. Chem.*, **2020**, *41*, 800–813. <https://doi.org/10.1002/jcc.26129>.
3. Patel, P.; Wang, J.; Wilson, A. K. Prediction of pK_as of Late Transition Metal Hydrides Via a QM/QM Approach. *J. Comput. Chem.*, **2020**, *41*, 171-183 <https://doi.org/10.1002/jcc.26057>. **Cover Article**
4. Eken, Y.; Patel, P.; Díaz, T.; Jones, M. R.; Wilson, A. K. SAMPL6 Host-Guest Challenge: Binding Free Energies via a Multistep Approach. *J. Comput. Aided. Mol. Des.* **2018**, *32* (10), 1097–1115. <https://doi.org/10.1007/s10822-018-0159-1>.
5. Obondi, C. O.; Lim, G. N.; Jang, Y.; Patel, P.; Wilson, A. K.; Poddutoori, P. K.; D'Souza, F. Charge Stabilization in High-Potential Zinc Porphyrin-Fullerene via Axial Ligation of Tetrathiafulvalene. *J. Phys. Chem. C* **2018**, *122* (25). <https://doi.org/10.1021/acs.jpcc.8b00028>.
6. Patel, P. and Wilson, A. K. Computational Chemistry Considerations in Catalysis: Regioselectivity and Metal-Ligand Dissociation *Catalysis Today* (Submitted)
7. Patel, P. and Wilson, A. K. Ab initio Composite Methodologies: Their Significance for the Chemistry Community. *J. Pure Appl. Chem.* (Submitted)
8. Patel, P.; Chung, J.; Bowman, M. A.; Ulusoy, I.; Wilson, A. K. Efficacy of DFT and ccCA in Obtaining Vibrational Potential Energy Surfaces *Phys. Chem. Chem. Phys.* (Submitted)
9. Patel, P.; Tomann, R.; Wilson, A. K. Active space coupled cluster methods within the correlation consistent Composite Approach *Chem. Phys. Lett.* (In preparation)
10. Patel, P. and Wilson, A. K. DLPNO-ccCA-TM: Applying DLPNO-ccCA to Transition Metal-Containing Species *Chem. Phys. Lett.* (In preparation)

CODES UTILIZED IN RESEARCH PROJECTS

· Gaussian, ORCA, NWChem, MolPro, VASP, PVSCF, Python, Mathematica, OCEAN, FDMNES, Quantum Espresso, ABINIT

POSTERS, PRESENTATIONS, AND SEMINARS

1. "Using the correlation consistent Composite Approach and Density Functional Theory in Generating Potential Energy Surfaces for Vibrational Properties" Prajay Patel, Joseph Chung, Max Aksel Bowman, Inga Ulusoy, Angela K. Wilson; Oral presentation; 51st Midwestern Theoretical Conference, Notre Dame University, South Bend, Illinois (June 2019)
2. "Computational Chemistry Considerations in Catalysis: Regioselectivity and Metal-Ligand Dissociation" Prajay Patel and Angela K. Wilson; Oral presentation; 40th Annual Symposium of the Michigan Chapter of the North American Catalysis Society, Dearborn, Michigan (May 2019)

3. "Expanding Applications of the correlation consistent Composite Approach using Local Methods" Prajay Patel and Angela K. Wilson; Poster presentation; 50th Midwestern Theoretical Conference, University of Chicago, Chicago, Illinois (June 2018)
4. "Utilizing the Domain-Based Local Methods to Expand the Size Limitations of the correlation consistent Composite Approach" Prajay Patel and Angela K. Wilson; Poster presentation; 39th Michigan Catalysis Society Symposium, Midland, Michigan (May 2018)
5. "Utilization of Local Methods to Reduce the Computational Cost Associated with ccCA" Prajay Patel and Angela K. Wilson; Poster presentation; 27th Austin Symposium of Molecular Structure and Dynamics, Dallas, Texas (March 2018)
6. "Utilization of Local Methods to Further Reduce Computational Cost within ccCA" Prajay Patel and Angela K. Wilson; Poster presentation; 58th Sanibel Symposium, St. Simons Island, Georgia (February 2018)
7. "Utilization of Methods to Further Reduce Computational Cost within ccCA" Prajay Patel and Angela K. Wilson; Poster presentation; 49th Midwestern Theoretical Conference, Michigan State University, East Lansing, Michigan (June 2017)
8. "pKa Prediction for Transition Metal Hydrides via a QM/QM Approach" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Poster presentation; 38th Annual Michigan Catalysis Society Spring Symposium, Ann Arbor, Michigan (May 2017)
9. "Prediction of pKa for Late Transition Metal Hydrides via a QM/QM Approach" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Poster presentation; Ninth Congress of the International Society for Theoretical Chemical Physics, Grand Forks, North Dakota (July 2016)
10. "A QM/QM Approach for the pKa of Late Transition Metal Hydrides" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Oral presentation; 49th ACS DFW Meeting-in-Miniature, Texas Woman's University, Denton, Texas (April 2016)
11. "Prediction of pKa via a QM/QM Approach" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Oral presentation; 251st ACS National Meeting, San Diego, California (March 2016)
12. "A QM/QM Approach for the pKa of Transition Metal Hydrides" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Poster presentation; 26th Austin Symposium of Molecular Structure and Dynamics, Dallas, Texas (March 2016)
13. "Quantification of pKa via a QM/QM Approach" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Oral presentation; Joint 71st ACS Southwestern/ 67th Southeastern Regional Meeting, Memphis, Tennessee (November 2015)
14. "The pKa Values of Transition Metal Hydrides in Acetonitrile: A DFT-ONIOM Study" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Oral presentation; Bonding Analysis Workshop, Phillips-Universität Marburg, Marburg, Germany (May 2015)
15. "Investigations of the Rhombohedral-to-cubic Transformation in Boron Nitride" Prajay Patel, and Peter Kroll; Oral presentation; 47th ACS DFW Meeting-in-Miniature, Texas Wesleyan University, Fort Worth, Texas (April 2014)
16. "Investigations of the r-BN to c-BN Transformation via First Principles Modeling" Christin P. Morrow, Prajay Patel and Peter Kroll; Oral presentation; 247th ACS National Meeting, Dallas, Texas (March 2014)
17. "Investigation of the rhombohedral-to-cubic transformation pathway in boron nitride," Prajay Patel, Miki Somosot, Anil Chourasia and Peter Kroll; Poster presentation; 247th ACS National Meeting, Dallas, Texas

(March 2014)

18. "Investigation of the rhombohedral-to-cubic transformation pathway in boron nitride," Prajay Patel, Miki Somosot, Anil Chourasia and Peter Kroll; Poster presentation; 69th ACS Southwest Regional Meeting, Waco, Texas (November 2013)
19. "Investigations of BN Transformation Pathways," Prajay Patel, Khoa Nguyen, Khanh Le, and Peter Kroll; Oral presentation; 46th ACS DFW Meeting-in-Miniature, Texas, A& M University- Commerce, Dallas, Texas (April 2013)

POSTERS, PRESENTATIONS, AND SEMINARS AT OWN INSTITUTION

1. "Computational Investigations into Vanadium K-edge XANES Spectroscopy: Orbital Analysis with Time-Dependent Density Functional Theory" Prajay Patel and Cong Liu; Poster presentation; 12th Postdoctoral Research and Career Symposium, Argonne National Laboratory, Argonne, Illinois (November 2019)
2. "DLPNO-ccCA: Utilization of the Domain-Based Local Pair Natural Orbital Methods within the correlation consistent Composite Approach" Prajay Patel; Seminar presented at Michigan State University, East Lansing, Michigan (February 2018)
3. "Comparative Study of Density Functionals on Ni-group Metal Hydrides" Prajay Patel, Jiaqi Wang, and Angela K. Wilson; Poster presentation; 9th Toulouse Graduate School Graduate Exposition, University of North Texas, Denton, Texas (March 2015)
4. "Investigations of Boron Nitride: From Soft to Hard Materials," Prajay Patel and Peter Kroll; Oral presentation; 10th Annual Celebration of Excellence by Students, Arlington, Texas (March 2014)
5. "Investigations of Boron Nitride: From Soft to Hard Materials," Prajay Patel, Khoa Nguyen, Khanh Le, and Peter Kroll; Poster; 9th Annual Celebration of Excellence by Students, Arlington, Texas (March 2013)

PROFESSIONAL SERVICE

Secretary, ACS Younger Chemists Committee
MSU Local Chapter

September 2018 - May 2019

PROFESSIONAL ACTIVITIES

ACS Younger Chemists Committee
MSU Local Chapter

2016 - 2019

- Organized, participated and led numerous chemistry-related community outreach events for K-12 and undergraduate students throughout the greater Lansing area.

North Texas Regional Science Bowl for the Department of Energy
College of Engineering, UTA

2013 - 2014

- Helped coordinate and manage the event for the high school division
- Organized the structure for the competition rooms

Engineering Saturday
College of Engineering, UTA

2011 - 2014

- Created a 90 minute demonstration targeted for K-12 students over material science engineering and chemistry

REFERENCES

1. Angela K. Wilson
John A. Hannah Distinguished Professor, MSU
akwilson@msu.edu
(517) 353-1111
2. Benjamin Levine
Associate Professor, MSU
levine@chemistry.msu.edu
(517) 353-1113
3. Inga Ulusoy
Research Associate, Universität Heidelberg
inga.ulusoy@pci.uni-heidelberg.de
+49/(0)6221/545208