Jark-Wah Andrew Wong

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Education

Ph.D. **Pennsylvania State University**, Chemical Engineering — Aug. 2019 to Aug. 2024
Dissertation Title: *Electrocatalysis at the Atomic Scale: Complexities at the Electrode-Electrolyte Interface*
Academic Minor: Computational Materials
Doctoral Advisor: Dr. Mike Janik
GPA: 3.87/4.0

B.S. **Texas A&M Unviversity**, Chemical Engineering, *magna cum laude* — Aug. 2015 to May 2019
Certification: Engineering Therapeutics Manufacturing
Dean's List: 2016-2019
GPA: 3.7/4.0

Professional Experience

Fritz Haber Institute of the Max Planck Society, Postdoctoral Fellow — Berlin, Germany
Advisor: Dr. Karsten Reuter — Present

- Investigating DFT models for predicting activation barriers of elementary electrocatalytic reactions

Pennsylvania State University, Graduate Research Assistant — University Park, PA, USA
Advisor: Dr. Mike Janik — Jan. 2020 to Aug. 2024

- Developed an analytical Grand Canonical DFT framework (aGC-DFT) to quantify the sensitivity of electrokinetic predictions based on the properties of the electrochemical double layer
- Investigating descriptors of elementary reaction kinetics across different late-transition metals and inner-sphere reactions
- Determining metal descriptors related to the specific adsorption of acetate and its implications on electrocatalysis

Collaborator: Dr. Adam Holewinski of University Colorado at Boulder

- Determining design principles of late-transition-metal alloys as catalysts for the electro-oxidation of biomass feedstocks

Collaborator: Dr. Matthias Waegele of Boston College

- Studying the distribution of TMA cations at the Au-electrolyte interface

Collaborator: Dr. Ezra Clark of the Pennsylvania State University

- Elucidating the origins of the activity,electronic, and stability promotion of Pd+Ge intermetallic electrocatalyst relative to Pd surface

Collaborator: Dr. Scott Milner of the Pennsylvania State University & Dr. Craig Plaisance of Louisiana State University

- Developed a DFT and Classical MD framework to comprehensively model solvation and electrification during specific alkali cation adsorption

Collaborator: Dr. Anne Co of Ohio State University

- Investigated surface coordination and cation effects on the CO_2 electrochemical reduction on Au surface

Collaborator: Dr. Bryan Goldsmith of the University of Michigan

- Elucidated and quantified the sensitivity of elementary reaction steps of CO electro-reduction on Cu surface due to the EDL properties

Collaborator: Dr. Chris Arges of Argonne National Laboratory

- Studied the roles of specifically adsorbed phosphonic and sulfonic anions within HER/HOR kinetics in electrochemical hydrogen pumps

Collaborator: CatalyzeH_2O LLC & Dr. Lauren Greenlee of XPRIZE

- Deduced the elementary reaction mechanism and design principles of electro-reduction catalysts of nitroaromatics: monometallic late-transition metals, bimetallics, and molecular Fe organic compounds as electrocatalysts

Lawrence Livermore National Laboratory, Computational Chemistry and Material Science Summer Intern — Livermore, CA, USA
Advisor: Dr. Sneha Akhade — May 2023 to Aug. 2023
Collaborator: Dr. Christopher Hahn of Lawrence Livermore National Laboratory

- Guided computational efforts between multi-disciplinary group for the design of biomass upgrading electrocatalysts
- Utilized DFT methods to study ligand and strain effects during the electro-oxidation of HMF oxidation on Ni oxide surface

Texas A&M University, Undergraduate Research Assistant — College Station, TX, USA
Advisor: Dr. Hung-Jen Wu — Dec. 2016 to May 2019

- Synthesized Ag-based catalysts through vapor deposition for sensor applications
- Characterized Ag deposited catalysts using Surface Enhanced Raman Spectroscopy

Research Interests

Energy Conversion and Storage
Renewable Energy
Environmental Remediation
Heterogeneous (Electro)Catalysis
Materials for Electrocatalysis
Materials for Photocatalysis
Surface Science
Properties of Interfaces
Computational Material Science
Electronic-Structure Calculations
Force Field Molecular Dynamics
Data Science
Machine Learning
Inclusive Education

Publications

Journal Articles

Google Scholar, *** = Equal Contribution**
The GitHub Repository of scripts and tools to reproduce data and utilize the methods based on my publications.

1. **Correlating Cation Distribution in the Electrochemical Double Layer with the Interfacial Fields** — Present
   Y. Hsu, ***A. J. Wong***, M. J. Janik, and M. Waegele
   (Manuscript in preparation)
2. **Electronic and Geometric Activity Promotion in PdGe Intermetallic Electrocatalyst** — Present
   M. Matalkeh, J. Li, ***A. J. Wong***, B. Vogt, M. J. Janik, and E. Clark
   (Manuscript in preparation)
3. **Model Consideration when Predicting Electrocatalytic Activation Barriers from Grand Canonical DFT** — Present
   A. J. Wong, D. Zhu, S. Chatterjee, R. Marks, and M. J. Janik
   (Manuscript in preparation)
4. **Descriptors of Electrocatalyzed Reaction Kinetics on Late-Transition-Metal Surfaces from Analytical Grand Canonical DFT** — Present
   A. J. Wong, N. Agrawal, D. Zhu, J. Li, and M. J. Janik
   (Manuscript in preparation)
5. **Electrode-electrolyte interfacial effects during specific cation adsorption on late-transition-metals using Density Functional Theory methods** — Present
   A. J. Wong, B. Tran, C. Plaisance, S. Milner, and M. J. Janik
   (Manuscript in preparation)
6. **Electrocatalytic Properties of an Fe Organometallic Complex and its Role in the Electro-Reduction of Nitroaromatic Compounds** — Present
   J. Miller, ***A. J. Wong***, and M. J. Janik
   (Manuscript in preparation)
7. **The Negative Reaction Order of CO during CO_2 Electroreduction on Au** — Present
   Z. Cui*, ***A. J. Wong****, M. J. Janik, and A. Co
   *(Manuscript in Review at the **Journal of the American Chemical Society**)*
8. **Cation effects on CO_2 reduction by single-crystal and polycrystalline gold electrodes under well-defined mass transport conditions** — Present
   Z. Cui*, ***A. J. Wong****, M. J. Janik, and A. Co
   *(Manuscript in Review at the **Angewandte Chemie**)*
9. **Sensitivity Analysis of Electrochemical Double Layer Approximations on Electrokinetic Predictions: Case Study for CO Reduction on Copper** — June 2024
   A. J. Wong*, B. Tran*, N. Agrawal, B. Goldsmith, and M. J. Janik
   Journal of Physical Chemistry C: Jens Nørskov Special Edition **DOI:**/10.1016/j.jcat.2024.115360

10. **An Efficient Approach to Compartmentalize Double Layer Effects on Kinetics of Interfacial Proton-Electron Transfer Reactions** — Feb. 2024
N. Agrawal, S. Maheswari, ***A. J. Wong***, and M. J. Janik
Journal of Catalysis **DOI:**/10.1016/j.jcat.2024.115360

11. **Deconvoluting Charge-Transfer, Mass Transfer, Ohmic Resistances in Phosphonic Acid-Sulfonic Acid Ionomer Binders Used in Electrochemical Hydrogen Pumps** — Oct. 2023
K. Arunagiri, ***A. J. Wong***, L. Briceno-Mena, H. Elsayed, J. Romagnoli, M. J. Janik,, and C. Arges
Energy and Environmental Science **DOI:**/10.1039/D3EE01776A

12. **Investigating the Electrocatalytic Reduction of 2,4,6-Tri-Nitro-Toluene (TNT) using Density Functional Theory Methods** — May 2023
A. J. Wong, J. Miller, B. Perdue, and M. J. Janik
Green Chemistry **DOI:**/10.1039/D3GC01144E

13. **Elementary mechanism for the electrocatalytic reduction of nitrobenzene on late-transition-metal surfaces from Density Functional Theory** — June 2022
A. J. Wong, J. Miller, and M. J. Janik
Chem Catalysis **DOI:**/10.1016/j.checat.2022.03.009

Book Chapter

1. **Density Functional Theory Methods for Electrocatalysis** — Present
N. Agrawal,K. Yeh ,S. Maheshwari, B. Tran, ***A. J. Wong***, and M. J. Janik
(Book chapter in Review)

Presentations

Oral Presentations

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1. **Theoretical Examination of Potential-Dependent CO Adsorption and Reaction on Copper Electrodes** — AIChE Fall 2024, Nov. 2024
B. Tran*, ***A. J. Wong*** N. Agrawal, M. J. Janik, and B. Goldsmith

2. **Invited: Electrode-Electrolyte Effects on Electrocatalytic Kinetics using a Compartmentalized DFT and Double-Layer Theory Approach** — ACS Spring 2024, Mar. 2024
A. J. Wong*, Z. Cui, A. Co, and M. J. Janik

3. **Multi-Scale Modeling of Electrocatalytic Processes within the Electrochemical Double Layer** — AIChE Fall 2023, Nov. 2023
A. J. Wong*, B. Tran, N. Agrawal, D. Zhu, S. Milner, and M. J. Janik

4. **Modeling Specific Alkali Cation Adsorption and Electrochemical Double-Layers with DFT and Classical MD** — NAM 28th 2023, June. 2023
A. J. Wong*, B. Tran, S. Milner, and M. J. Janik

5. **Incorporating Electrode-Electrolyte Interfacial Effects on the Specific Adsorption of Ions on Late Transition Metal Surfaces Using a Combined DFT/FF-MD Approach** — AIChE Fall 2022, Nov. 2022
A. J. Wong*, B. Tran, N. Agrawal, S. Milner, and M. J. Janik

6. **A Combined Classical MD and DFT Approach for Modeling Ionic Adsorption on Metal Electrodes with Explicit Description of the Electrical Double Layer** — AIChE Fall 2022, Nov. 2022
   B. Tran*, ***A. J. Wong***, N. Agrawal, S. Milner, and M. J. Janik
7. **Incorporating Electrode-Electrolyte Interfacial Effects on the Specific Adsorption of Alkali Cations on Late Transition Metal Surfaces Using a Combined DFT and FF-MD Approach** — PSU ChE Symposium, Sept. 2022
   A. J. Wong*, B. Tran, N. Agrawal, S. Milner, and M. J. Janik
8. **Elementary Mechanisms of the Electrocatalytic Reduction of Nitroaromatics on Late Transition Metal Surfaces using Density Functional Theory Methods** — ACS Spring 2022, Mar. 2022
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik
9. **Mechanistic Studies on the Electrocatalytic Reduction of Nitroaromatic Compounds** — AIChE Fall 2021, Nov. 2021
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik

Poster Presentations

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1. **Modeling Electrode-Electrolyte Interfacial Effects and Specific Alkali Metal Cation Adsorption Using DFT/FF-MD Approach** — AIChE Fall 2023, Nov. 2023
   A. J. Wong*, B. Tran, S. Milner, and M. J. Janik
2. **Modeling Electrode-Electrolyte Interfacial Effects and Specific Alkali Metal Cation Adsorption Using DFT/FF-MD Approach** — 2023 Catalysis Club, May. 2023
   A. J. Wong*, B. Tran, D. Zhu, S. Milner, and M. J. Janik
3. **Modeling Electrode-Electrolyte Interfacial Effects and Specific Alkali Metal Cation Adsorption Using DFT/FF-MD Approach** — PCCS Symposium, May 2023
   A. J. Wong*, B. Tran, D. Zhu, S. Milner, and M. J. Janik
4. **Investigating the Electrocatalytic Reduction of 2,4,6-Tri-Nitro-Toluene across Late Transition Metal Surfaces Using Density Functional Theory Methods** — AIChE Fall 2022, Nov. 2022
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik
5. **Elementary Mechanism for the Electrocatalytic Reduction of Nitrobenzene on Late Transition Metal Surfaces from Density Functional Theory Methods** — PSU ChE Symposium, Sept. 2022
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik
6. **Elementary Mechanism for the Electrocatalytic Reduction of Nitrobenzene on Late Transition Metal Surfaces from Density Functional Theory Methods** — PCCS Symposium, Aug. 2022
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik
7. **Electrocatalytic Reduction of Nitrobenzene by Iron-Salen Ligand Complexes** — AIChE Fall 2021, Nov. 2021
   J. Miller*, B. Perdue, ***A. J. Wong***, and M. J. Janik
8. **Elementary mechanism for the Electrocatalytic Reduction of Nitrobenzene on Late Transition Metal Surfaces from Density Functional Theory Methods** — PSU ChE Symposium, Oct. 2021
   A. J. Wong*, J. Miller, B. Perdue, and M. J. Janik

Teaching & Work Experiences

Graduate Teaching Assistant, The Pennsylvania State University — University Park, PA, USA
Course: ChE 535: Graduate Chemical Reaction Engineering — Aug. 2023 to Dec. 2023

- Lectured advantaced graduate chemical reaction energineering and catalytic principles to over 30 first-year graduate students
- Provided mentorship for first-year graduate students in Ph.D. advisor and research lab selection

Graduate Teaching Intern and Assistant, The Pennsylvania State University — University Park, PA, USA
Course: ChE 430: Undergraduate Chemical Reaction Engineering — Aug. 2023 to Dec. 2023

- Led lectures of over 70 students through a "flipped classroom", where students collaboratively solved problems and consulted the TA for reinfornced learning
- Designed lecture and exam problems to test student's knowledge on applicable problems in chemical reactor design and catalysis
- Organized multiple in-person and remote weekly office hours and monthly review sessions

Hardware and Software Lab Manager, The Pennsylvania State University — University Park, PA, USA
Jan. 2020 to Aug. 2024

- Manage Janik lab hardware for efficient research through collaboration with PSU IT department
- Supervise supercomputing allocation usage across clusters for over 16 lab students
- Design and update the Mike Janik lab website

Undergraduate Teaching Assistant, Texas A&M University — College Station, TX, USA
Course: CHEN 204: Chemical Reaction Engineering — Aug. 2018 to Dec. 2018

- Managed weekly recitation of over 200 students to teach fundamental mass balance and chemical engineering principles through group practice problems

Private Lesson Teacher, Frisco Centennial High School — Frisco, TX, USA
July 2015 to Aug. 2016

- Taught music and leadership principles to over 50 students
- Managed lesson plans during leadership camp encompassing over 200 students

Scientific Community Service

Scientific Journal Peer Reviewer for the Journal of Catalysis — Aug. 2024 - Present

Judge for The PSU 2024 Undergraduate Exhibition — April 2024

Volunteer at the NAM28 — June 2023

Extracurricular and Leadership Activities

Penn State Chemical Engineering Graduate Student Association — University Park, PA, USA
Graduate Student Mentor Mentor — Aug. 2019 to Aug. 2024

- Train and co-supervise undergraduate and Ph.D. students in using DFT methods for electrocatalysis, where both undergrads respectively were awarded NSF Fellowship and full-time job offer at Chemours
- Lead weekly electrochemistry meetings to facilitate collaboration for Ph.D. students across departments
- Advise theoretical electrocatalysis students in Mike Janik lab in research direction and writing a paper together regarding best modeling practices
- Mentoring first year Ph.D. students through courses and Ph.D. work, where one student was awarded the best qualifying oral exam in 2022 under my supervision

American Institute of Chemical Engineers College Station, TX, USA
Vice President, Publicity Mar. 2017 to Mar. 2019

- Awarded best national AIChE student chapter during tenure
- Coordinated record high meeting and workshop attendances for prospective and current ChE students
- Chaired engaging session at the SPARK Conference to teach middle and high school students about careers and principles in engineering

Omega Chi Epsilon Chemical Engineering Honor Society College Station, TX, USA
Mentor Dec. 2017 to Mar. 2019

- Invited to the organization to mentor engineering students due to outstanding academic achievement
- Assisted in annual Big Event to perform volunteer work for the community in Bryan, TX

Honors and Awards

ACS ChemCatBio Award Mar. 2024

NAM28 Kokes Award Feb. 2023

Dean's List Jan. 2016 to May 2019

Technical Skills

Languages: Proficient in Python, Bash, TeX, MATLAB, Vim, Wolfram Language, and R

Softwares and Skills:

Density Functional Theory	Materials Project
Vienna Ab Initio Software (VASP)	VESTA
Gaussian16	Wolfram Alpha
Atomic Simulation Environment (ASE)	MATLAB
GROMACS	ApacheSpark
Classical Molecular Dynamics	TensorFlow
Visual Studio	R
Amsterdam Modeling Suite	Bash Scripting

Hobbies

Photography	Basketball
Playing Guitar	Tennis
Video games	Board Games
Traveling	Cooking
Exploring New Foods	Visting Museums
Producing Music	Playing Jazz Music
Yoga	Hanging out with my Cat