Leanne D. Chen

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Summary

Interests	Computational chemistry, catalysis, electrochemistry, materials and interfaces Energy storage, energy transformation, sustainability
Skills	Python, LaTeX, Atomic Simulation Environment, Matplotlib, VMD

Academic Appointments

2020–	**University of Guelph**, Guelph, Ontario Assistant Professor, Department of Chemistry
2017–2019	**California Institute of Technology**, Pasadena, California Postdoctoral Scholar, Division of Chemistry and Chemical Engineering *Advisor: Thomas F. Miller III*

Education

2012–2017	**Stanford University**, Stanford, California PhD, Physical Chemistry *Advisor: Jens K. Nørskov*
2008–2012	**Queen's University**, Kingston, Ontario BSc Honours with Distinction, Chemistry *Advisors: Nicholas J. Mosey and Suning Wang*
2004–2008	**Talented Offerings for Programs in the Sciences (TOPS)**, Toronto, Ontario

Publications

* denotes equal contribution

17 Gauthier, J. A.; **Chen, L. D.**; Bajdich, M.; Chan, K. Implications of the Fractional Charge of Hydroxide at the Electrochemical Interface. *PCCP* **2020**, *Advance Article*. Link

16 Ringe, S.; Morales-Guio, C. G.; **Chen, L. D.**; Fields, M.; Jaramillo, T. F.; Hahn, C.; Chan, K. Double layer charging driven CO_2 adsorption limits the rate of electrochemical CO_2 reduction on Au. *Nat. Commun.* **2020**, *11*, 33. Link

15 Gauthier, J. A.; Fields, M.; Bajdich, M.; **Chen, L. D.**; Sandberg, R. B.; Chan, K.; Nørskov, J. K. Electron Transfer to CO_2 during Adsorption at the Metal | Solution Interface. *J. Phys. Chem. C* **2019**, *123*, 29278–29283. **Link**

14 **Chen, L. D.**; Bajdich, M.; Martirez, J. M. P.; Krauter, C. M.; Gauthier, J. A.; Carter, E. A.; Luntz, A. C.; Chan, K.; Nørskov, J. K. Understanding the Apparent Fractional Charge of Protons in the Aqueous Electrochemical Double Layer. *Nat. Commun.* **2018**, *9*, 3202. **Link**

13 *Kirk, C.; ***Chen, L. D.**; *Siahrostami, S.; Karamad, M.; Bajdich, M.; Voss, J.; Nørskov, J. K.; Chan, K. Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene. *ACS Cent. Sci.* **2017**, *3*, 1286–1293. **Link**

12 Resasco, J.; **Chen, L. D.**; Clark, E. L.; Tsai, C.; Hahn, C.; Jaramillo, T. F.; Chan, K.; Bell, A. T. Promoter Effects of Alkali Metal Cations on the Electrocatalytic Reduction of Carbon Dioxide. *J. Am. Chem. Soc.* **2017**, *139*, 11277–11287. **Link**

11 Gauthier, J. A.; Dickens, C. F.; **Chen, L. D.**; Doyle, A. D.; Nørskov, J. K. Solvation Effects for Oxygen Evolution Reaction Catalysis on IrO_2 (110). *J. Phys. Chem. C* **2017**, *121*, 11455–11463. **Link**

10 Fields, M.; Tsai, C.; **Chen, L. D.**; Abild-Pedersen, F.; Nørskov, J. K.; Chan, K. Scaling Relations for Adsorption Energies on Doped Molybdenum Phosphide Surfaces. *ACS Catal.* **2017**, *7*, 2528–2534. **Link**

9 **Chen, L. D.**; Urushihara, M.; Chan, K.; Nørskov, J. K. Electric Field Effects in Electrochemical CO_2 Reduction. *ACS Catal.* **2016**, *6*, 7133–7139. **Link**

8 Tsai, C.; Lee, K.; Yoo, J. S.; Liu, X.; Aljama, H.; **Chen, L. D.** et al. Direct Water Decomposition on Transition Metal Surfaces. *Catal. Lett.* **2016**, *146*, 718–724. **Link**

7 **Chen, L. D.**; Nørskov, J. K.; Luntz, A. C. Theoretical Limits to the Anode Potential in Aqueous Mg–Air Batteries. *J. Phys. Chem. C* **2015**, *119*, 19660–19667. **Link**

6 **Chen, L. D.**; Nørskov, J. K.; Luntz, A. C. Al–Air Batteries: Fundamental Thermodynamic Limitations from First-Principles Theory. *J. Phys. Chem. Lett.* **2014**, *6*, 175–179. **Link**

5 Neverov, A. A.; **Chen, L. D.**; George, S.; Simon, D.; Maxwell, C. I.; Brown, R. S. A mechanistic study of the $[La_2(OCH_3)_2]^{4+}$- and [(1,5,9-triazacyclododecane):Zn:(OCH_3)]$^+$-catalyzed methanolysis of carbonates: possible application for the recycling of bisphenol A polycarbonates. *Can. J. Chem.* **2013**, *91*, 1139–1146. **Link**

4 Wang, N.; Ko, S.-B.; Lu, J.-S.; **Chen, L. D.**; Wang, S. Tuning the Photoisomerization of an NC-Chelate Organoboron Compound with a Metal–Acetylide Unit. *Chem. Eur. J.* **2013**, *19*, 5314–5323. **Link**

3 Rao, Y.-L.; Amarne, H.; **Chen, L. D.**; Brown, M. L.; Mosey, N. J.; Wang, S. Photo- and Thermal-induced Multistructural Transformation of 2-Phenylazolyl Chelate Boron Compounds. *J. Am. Chem. Soc.* **2013**, *135*, 3407–3410. Link

2 Rao, Y.-L.; **Chen, L. D.**; Mosey, N. J.; Wang, S. Stepwise Intramolecular Photoisomerization of NHC-Chelate Dimesitylboron Compounds with C–C Bond Formation and C–H Bond Insertion. *J. Am. Chem. Soc.* **2012**, *134*, 11026–11034. Link

1 Sun, C.; Hudson, Z. M.; **Chen, L. D.**; Wang, S. Double Cyclization/Aryl Migration Across an Alkyne Bond Enabled by Organoboryl and Diarylplatinum Groups. *Angew. Chem. Int. Ed.* **2012**, *51*, 5671–5674. Link

Invited Seminars

2020 **Department of Chemistry, University of Waterloo**, Waterloo, Ontario
"Atomic-Scale Computational Insight into Electrochemical Reactions: from Mechanistic Understanding to Materials Engineering"

2019 **Computational Catalysis & Materials Design Lab, University of Seoul**, Seoul, South Korea
"Understanding the Apparent Fractional Charge of Protons in the Aqueous Electrochemical Double Layer"

2019 **Complex Molecular-Systems Multiscale Design Lab, KAIST**, Daejeon, South Korea
"Atomic-Scale Computational Insight into Electrochemical Reactions: from Mechanistic Understanding to Materials Engineering"

2019 **Lawrence Livermore National Laboratory**, Livermore, California
"Exploring the Potential of Metal-Doped Graphene as Improved Electrocatalysts for CO_2 Reduction Using Embedded Mean-Field Theory"

2019 **Toyota Research Institute**, Los Altos, California
"Understanding the Apparent Fractional Charge of Protons in the Aqueous Electrochemical Double Layer"

2019 **257th American Chemical Society National Meeting**, Orlando, Florida
"Understanding the Apparent Fractional Charge of Protons in the Aqueous Electrochemical Double Layer"

2019 **Department of Chemistry, University of Guelph**, Guelph, Ontario
"Atomic-Scale Computational Insight into Electrochemical Reactions: from Mechanistic Understanding to Materials Engineering"

2019 **Department of Chemical Engineering, University of Colorado Boulder**, Boulder, Colorado
"Atomic-Scale Computational Insight into Electrochemical Reactions:
from Mechanistic Understanding to Materials Engineering"

2019 **Department of Chemical Engineering, University of Delaware**, Newark, Delaware
"Atomic-Scale Computational Insight into Electrochemical Reactions:
from Mechanistic Understanding to Materials Engineering"

2019 **Department of Chemistry, York University**, Toronto, Ontario
"Atomic-Scale Computational Insight into Electrochemical Reactions:
from Mechanistic Understanding to Materials Engineering"

2017 **Dynamics at Surfaces Gordon Research Conference**, Newport, Rhode Island
"First-Principles Modeling of the Electrochemical Interface"

2017 **Department of Chemical Engineering, MIT**, Cambridge, Massachusetts
"Electrochemical Energy Transformation Processes: An Atomistic Perspective"

2016 **Department of Electrical Engineering, University of Toronto**, Toronto, Ontario
"Electrochemical Energy Transformation Processes: An Atomistic Perspective"

Awards and Distinctions

2018 **Gordon Research Seminar in Catalysis Presentation Award**
One of ten selected seminars awarded to graduate students and postdoctoral scholars
2017 **North American Catalysis Society Kokes Award**
Merit-based travel award for graduate students attending the North American Catalysis Meeting
2013 **NSERC Alexander Graham Bell Canada Graduate Scholarship (CGS-D3)**
Offered to the top-ranked Postgraduate Scholarship (Doctoral) applicants (declined for PGS-D3)
2012 **NSERC Alexander Graham Bell Canada Graduate Scholarship (CGS-M)**
Offered to the top-ranked Postgraduate Scholarship (Master's) applicants (declined for PGS-M)
2012 **Ontario Graduate Scholarship** *(declined)*
2012 **DAAD Professional Research Internships in Science and Engineering**
Received funding for an industrial summer research internship in Germany
2012 **NSERC Undergraduate Student Research Award** *(declined)*
2012 **Walter MacFarlane Smith Prize in Chemistry for Best Thesis**
Awarded annually to a graduating Honours Chemistry student in the Faculty of Arts and Science on the basis of outstanding achievement for a research project
2012 **Best Presentation Award, Physical Chemistry Division**
40th Southern Ontario Undergraduate Chemistry Conference
2011 **Dean's Honour List with Distinction** *top 3% of students ranked by GPA*
2011 **NSERC Undergraduate Student Research Award**

Teaching

2018 **The Dow Chemical Company**, Midland, Michigan
Gave a lecture-style software demonstration to industrial collaborators and helped integrate our in-house code within their catalyst discovery workflow

2015–2017 **SUNCAT Center for Interface Science and Catalysis**, Stanford, California
Gave hands-on guidance to first- and second-year PhD students on project design and direction; co-author on two publications as mentor

2012–2014 **Stanford University**, Stanford, California
As a Teaching Assistant, held weekly office hours, graded assignments and exams, created problem sets, gave laboratory demonstrations, and held weekly lecture-style sections depending on the course taught
CHEM 036: Organic Chemistry Laboratory I
CHEM 131: Organic Polyfunctional Compounds
CHEM 181: Biochemistry I
CHEM 275: Topics in Molecular Modeling (graduate course)

Service

2015–Now Referee for *ACS Omega* (1), *Chem. Sci.* (4), *Energy Environ. Sci.* (8), *J. Mater. Chem. A* (2), *Mol. Syst. Des. Eng.* (1), *Phys. Chem. Chem. Phys.* (2), North American Catalysis Meeting (2019)
2019 Reviewer, Institution Level Grant
2019 Breakout Session Leader, JCAP All-Hands Meeting
2017 Graduate Representative on Faculty Search Committee (Stanford University)
2012 Undergraduate Representative on Tenure Committee (Queen's University)

Select Contributed Presentations

2018 **Joint Center for Artificial Photosynthesis Theory Meeting**, Menlo Park, California
"Exploring the Potential of Metal-Doped Graphene as Improved Electrocatalysts for CO_2 Reduction Using Embedded Mean-Field Theory"

2018 **Gordon Research Seminar on Catalysis**, New London, New Hampshire
"Exploring the Potential of Metal-Doped Graphene as Improved Electrocatalysts for CO_2 Reduction Using Embedded Mean-Field Theory" *(Selected Talk)*

2018 **3rd Annual Southern California Theoretical Chemistry Conference**, Pasadena, California
"Metal-Doped Graphene for CO_2 Electroreduction with Quantum Embedding Methods" *(Poster)*

2018 **American Physical Society March Meeting**, Los Angeles, California
"Exploring the Potential of Metal-Doped Graphene as Improved Electrocatalysts for CO_2 Reduction Using Embedded Mean-Field Theory"

2018 **Berkeley Statistical Mechanics Meeting**, Berkeley, California
"Metal-Doped Graphene for CO_2 Electroreduction with Quantum Embedding Methods" *(Poster)*

2017 **The Electrode Potential in Electrochemistry Workshop**, Günzburg, Germany
"Metal-Doped Graphene for CO_2 Electroreduction with Quantum Embedding Methods" *(Poster)*

2017 **Caltech Seminar Day**, Pasadena, California
"Quantum Embedding Methods for Reactions on Graphene" *(Poster)*

2017 **25th North American Catalysis Society Meeting**, Denver, Colorado
"The Charge of an Ion in the Outer Helmholtz Plane"

2017 **253rd American Chemical Society National Meeting**, San Francisco, California
"The Charge of an Ion in the Outer Helmholtz Plane"

2016 **AIChE Annual Meeting**, San Francisco, California
"*Ab Initio* Insights into the Electrochemical Double Layer"

2016 **99th Canadian Society for Chemistry Conference and Exhibition**, Halifax, Nova Scotia
"Electric Field Effects in Electrochemical CO_2 Reduction"

2015 **4th Annual ReLiable Metal–Air Workshop**, Copenhagen, Denmark
"An Atomistic Description of Anode Reactions in Aqueous Mg–Air Batteries"

2015 **American Physical Society March Meeting**, San Antonio, Texas
"Al–Air Batteries: Fundamental Thermodynamic Limitations from First-Principles Theory"

2014 **3rd Annual ReLiable Metal–Air Workshop**, Copenhagen, Denmark
"DFT Studies of the Fundamental Mechanisms in Aqueous Mg–O_2 and Al–O_2 Batteries"

2014 **CAMD Summer Institute**, Lyngby, Denmark
"Density Functional Theory Studies of Aqueous Mg-Air and Al-Air Batteries" *(Poster)*

2013 **AIChE Annual Meeting**, San Francisco, California
"Toward High Specific Energy Metal–Air Batteries in Vehicle Propulsion Applications"

2013 **2nd Annual ReLiable Metal–Air Workshop**, Copenhagen, Denmark
"*Ab Initio* Investigations of Mg–Air and Al–Air Batteries"