Jianli Cheng, Ph.D.

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EDUCATION

Ph.D. **Chemical Engineering** **University of California, San Diego** July 2018

Thesis: First-Principles Study of Two-Dimensional Electron Gas in Perovskite Oxide Heterostructures

M.S. **Chemical Engineering** **Rutgers University** June 2014

Thesis: Morphological transformations in polymer brushes in binary mixtures: DPD study

RESEARCH EXPERIENCE

Postdoctoral Researcher, Lawrence Berkeley National Laboratory, Berkeley 2018-present

Advisor: Prof. Kristin A. Persson

- Developing materials design principles of amorphous electrode coatings for Li-ion batteries using data-driven materials discovery and machine learning.
- Developing 3D targeted doping to stabilize low-/no-Co cathode materials for next-generation Li-ion batteries using first-principles calculations, cluster expansion and Monte Carlo simulations.

Ph.D. Student, University of California, San Diego 2014-2018

Advisor: Prof. Kesong Yang

- Developed a high-throughput computational scheme to screen for perovskite oxide heterointerfaces with two-dimensional electron systems.
- Developed a Python library, aimsgb, for building periodic grain boundary models.

Master Student, Rutgers University, New Brunswick 2012-2014

Advisor: Prof. Alexander V. Neimark

- Investigated adhesion of nanoparticles to polymer brushes and morphological transformations in polymer brushes in binary mixtures using dissipative particle dynamics simulation.

AWARDED RESEARCH GRANT

Jan. 2021-Oct. 2022 *Stabilizing the interface between cathode and solid electrolyte through theory guided cathode coating selection for all-solid-state batteries*
Lawrence Berkeley National Laboratory
CalTestBed Initiative, $280,000
Role: Draft the entire research proposal. Collaborate with Coreshell Technologies, Inc. to design cathode coatings for all-solid-state batteries.

TEACHING EXPERIENCE

Graduate Teaching Assistant, University of California, San Diego Fall 2014
Course: Chemical Reaction Engineering
Responsibilities: Hold office hours and grade homework and exams

Graduate Teaching Assistant, University of California, San Diego Spring 2015
Course: Engineering Computation Using MATLAB
Responsibilities: Hold office hours and occasionally give class lectures

Graduate Teaching Assistant, University of California, San Diego Fall 2015
Course: Separation Processes
Responsibilities: Hold office hours, class discussions and occasionally give class lectures

PUBLICATIONS

26 total journal publication; **~940** Google Citations (October 2022)

1. **J. Cheng** and K. Persson, Enhancing Structural Stability of Ni-rich Cathodes using Doping Engineering, submitted.
2. **J. Cheng**, Kara D. Fong, Kristin A. Persson, *Materials Design Principles of Amorphous Cathode Coatings for Lithium-ion Battery Applications*, **J. Mater. Chem. A**, 10, 22245, (**2022**).
3. Y. Zhang†, **J. Cheng**†, Y. Tian, G. Ceder, K. Persson, M.C. Scott, *Oxygen Transport through Conformal Cathode Coatings in Solid State Battery*, **Nat. Commun.**, **in revision**.
4. J. Burns, B. Ouyang, **J. Cheng**, M. Horton, M. Siron, O. Andriuc, R. Yang, G. Ceder, and K. Persson, *Equilibrium Particle Shape and Surface Chemistry of Disordered Li-Excess, Mn-Rich Li-ion Cathodes through First-Principles Modeling*, **Chem. Mater.**, (**2022**)
5. **J. Cheng**, E. Sivonxay, and K. Persson, *Evaluation of Amorphous Oxide Coatings for High-voltage Li-ion Battery Applications using a First-Principles Framework*, **ACS Appl. Mater. Interfaces**, 12, 31, 35748, (**2020**).
6. **J. Cheng**, L. Mu, C. Wang, Z. Yang, H. Xin, F. Lin, and K. Persson, *Enhancing Surface Oxygen Retention through Theory-guided Doping Selection in Layered Ni-rich Cathodes for Next-generation Lithium-ion Batteries*, **J. Mater. Chem. A**, 8, 23293, (**2020**)
7. Y. Wang, Z. Zhang, **J. Cheng**, Q. Zhang, W. Tang and K. Yang, *Creating a two-dimensional hole gas in a polar/polar $LaAlO_3/KTaO_3$ perovskite heterostructure*, **J. Mater. Chem. C**, 8, 14230, (**2020**).
8. B. Xia, **J. Cheng**, M. Arengo, N. Rajput, Y. Janssen, J. Neilson, K. Persson, and J. Simonson, *Trigonal polymorph of Li_2MnO_3*, **Phys. Rev. Materials**, 4, 085401, (**2020**).
9. J. Ding, **J. Cheng**, F. Dogan, Y. Li, W. Lin, Y. Yao, A. Manchon, K. Yang, T. Wu, *Two-Dimensional Electron Gas at Spinel/Perovskite Interface: Interplay between Polar Catastrophe and Structural Defects*, **ACS Appl. Mater. Interfaces**, 12, 42982, (**2020**).
10. L. Li, **J. Cheng**, H. Wang, J. Huang, X. Gao, X. Wang, S. Misra, B. Zhang, J. Jian, A. Chen, P. Lu, X. Qian, K. Yang, and H. Wang, *Interfacial Engineering Enabled Novel Bi-Based Layered Oxide Supercells with Modulated Microstructures and Tunable Physical Properties*, **Cryst. Growth Des.**, 19, 7088, (**2019**).
11. S. Naziar, S. Jiang, **J. Cheng**, and K. Yang, *Enhanced Interfacial Perpendicular Magnetic Anisotropy in Fe/MgO Heterostructure via Interfacial Engineering*, **Appl. Phys. Lett.**, 114, 072407, (**2019**).
12. L. Li, P. Boullay, **J. Cheng**, P. Lu, X. Wang, G. Steciuk, J. Huang, J. Jian, X. Gao, B. Zhang, S. Misra, X. Zhang, K. Yang, and H. Wang, *Self-Assembled Two-Dimensional Layered Oxide Supercells with Modulated Layer Stacking and Tunable Physical Properties*, **Mater. Today Nano**, 6, 100037, (**2019**).
13. **J. Cheng**, J. Luo and K. Yang, *Aimsgb: An Algorithm and Open-Source Python Library to Generate Periodic Grain Boundary Structures*, **Comput. Mater. Sci.**, 155, 92, (**2018**).
14. **J. Cheng** and K. Yang, *Design of two-dimensional electron gas systems via polarization discontinuity from large-scale first-principles calculations*, **J. Mater. Chem. C**, 6, 6680, (**2018**).
15. Y. Wang, **J. Cheng**, M. Behtash, W. Tang, J. Luo, and K. Yang, *First-Principles Studies of Polar Perovskite $KTaO_3$ Surfaces: Structural Reconstruction, Charge Compensation, and Stability Diagram*, **Phys. Chem. Chem. Phys.**, 20, 18515, (**2018**).
16. **J. Cheng**, Yaqin Wang, Jian Luo, and Kesong Yang, *δ-Doping Effects on Electronic and Energetic Properties of $LaAlO_3/SrTiO_3$ Heterostructure: First-Principles Analysis of 23 Transition-Metal Dopants*, **Adv. Mater. Interfaces**, 4, 1700579, (**2017**).
17. **J. Cheng**, J. Luo, and K. Yang, *Comparison Studies of Interfacial Electronic and Energetic Properties of $LaAlO_3/TiO_2$ and $TiO_2/LaAlO_3$ Heterostructures from First-Principles Calculations,* **ACS Appl. Mater. Interfaces**, 9, 7682, (**2017**).
18. P. Joo, **J. Cheng**, and K. Yang, *Size Effects and Odd-Even Effects in the MoS_2 Nanosheets: First-*

Principles Studies, **Phys. Chem. Chem. Phys.**, 19, 29927, (**2017**).

19. **J. Cheng**, S. Nazir, and K. Yang, *First-Principles Prediction of Two-Dimensional Electron Gas Driven by Polarization Discontinuity in Nonpolar/Nonpolar $AHfO_3/SrTiO_3$ (A=Ca, Sr, and Ba) Heterostructures,* **ACS Appl. Mater. Interfaces**, 8, 31959, (**2016**).
20. Y. Wang, W. Tang, **J. Cheng**, M. Behtash, and K. Yang, *Creating Two-Dimensional Electron Gas in Polar/Polar Perovskite Oxide Heterostructures: First-Principles Characterization of $LaAlO_3/A^+B^{5+}O_3$,* **ACS Appl. Mater. Interfaces**, 8, 13659, (**2016**).
21. L. Liu, Y. Jiang, H. Zhao, J. Chen, **J. Cheng**, K. Yang, and Y. Li, *Engineering Ti^{3+} Sites and Co-exposed {001} and {101} Facets in TiO_2 Nanocrystals for Enhanced CO_2 Photoreduction under Visible Light*, **ACS Cata.**, 6, 1097, (**2016**).
22. Y. Wang, W. Tang, **J.Cheng**, S. Nazir, K. Yang, *High-mobility two-dimensional electron gas in $SrGeO_3$-and $BaSnO_3$-based perovskite oxide heterostructures: an ab initio study.* **Phys. Chem. Chem. Phys.**, 18 (46), 31924, (**2016**).
23. K. Yang, S. Nazir, M. Behtash, and **J. Cheng**, *High-Throughput Design of Two-Dimensional Electron Gas Systems Based on Polar/Nonpolar Perovskite Oxide Heterostructures,* **Sci. Rep.** 6, 34667, (**2016**).
24. S. Nazir, M. Behtash, **J. Cheng**, J. Luo, and K. Yang, *Nb and Ta Layer Doping Effects on the Interfacial Energetics and Electronic Properties of LaAlO3/SrTiO3 Heterostructure: First-Principles Analysis,* **Phys. Chem. Chem. Phys.**, 18, 2379, (**2016**).
25. S. Nazir, **J. Cheng**, and K. Yang, *Creating Two-Dimensional Electron Gas in Nonpolar/Nonpolar Oxide Interface via Polarization Discontinuity: First-Principles Analysis of $CaZrO_3/SrTiO_3$ Heterostructure* **ACS Appl. Mater. Interfaces**, 8, 390, (**2016**).
26. S. Nazir, **J. Cheng**, M. Behtash, J. Luo, and K. Yang, *Interface Energetics and Charge Carrier Density Amplification by Sn-doping in $LaAlO_3/SrTiO_3$ Heterostructure*, **ACS Appl. Mater. Interfaces**, 7, 14294, (**2015**).
27. **J. Cheng**, A. Vishnyakov and A.V. Neimark, *Adhesion of Nanoparticles to Polymer Brushes Studied with the Ghost Tweezers Method*, **J. Chem. Phys.**, 142, 034705 (**2015**).
28. **J. Cheng**, A. Vishnyakov and A.V. Neimark, *Morphological Transformations in Polymer Brushes in Binary Mixtures: DPD study*, **Langmuir**, 30, 12932 (**2014**).

PRESENTATIONS

1. *"Computational Design of Surface Coating and Targeted Doping for Li-ion Batteries."* Telluride Science Research Center, Colorado, 2022. (Oral, Invited)
2. *"Materials Design Principles of Amorphous Cathode Coatings for Lithium-Ion Battery Applications."* Berkeley Electrochemistry Seminar Series, Berkeley, California, 2022. (Oral)
3. *"Materials Design Principles of Amorphous Cathode Coatings for Lithium-Ion Battery Applications."* ICMCTF, San Diego, California, 2022. (Oral, Invited)
4. *"Materials Design Principles of Amorphous Cathode Coatings for Lithium-Ion Battery Applications."* MRS Spring Meeting, Honolulu, Hawai'i, 2022. (Oral)
5. *"Computational Design of Surface Coating and Targeted Doping for Li-ion Cathode Materials."* Faculty Candidate Seminar, San Diego State University, 2022. (Oral, Invited)
6. *"Evaluation of Amorphous Oxide Coatings for High-Voltage Li-Ion Battery Applications Using a First-Principles Framework."* ECS PRiME (virtual), 2020. (Oral)
7. *"Investigate Li Intercalation Stability of Ni-Rich Cathodes from First-Principles."* Berkeley Electrochemistry Seminar Series, Berkeley, California, 2019. (Oral)
8. "*GBMaker: an efficient and open-source Python library for making grain boundaries*." APS March Meeting, Los Angeles, California, 2018. (Oral)

9. "*δ-Doping Effects on Electronic and Energetic Properties of $LaAlO_3/SrTiO_3$ Heterostructure: First-Principles Analysis of 23 Transition-Metal Dopants*." Electronic and Advanced Materials, Orlando, Florida, 2018. (Oral)
10. "*First-Principles Prediction of Two-Dimensional Electron Gas Driven by Polarization Discontinuity in Nonpolar/Nonpolar $AHfO_3/SrTiO_3$ (A = Ca, Sr, and Ba) Heterostructures*." APS March Meeting, New Orleans, Louisiana, 2017. (Oral)
11. "*High-Throughput Design of Two-Dimensional Electron Gas Systems Based on Polar/Nonpolar Perovskite Oxide Heterostructures*" MRS Spring Meeting, Phoenix, Arizona, 2016. (Poster)