



Jianli Cheng, Ph.D.
Lawrence Berkeley National Laboratory, Berkeley, CA
jianlicheng@lbl.gov



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**, Accepted, **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 LaAlO₃/KTaO₃ 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 Li₂MnO₃*, **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*, **Materials 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 KTaO₃ 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 LaAlO₃/SrTiO₃ Heterostructure: First-Principles Analysis of 23 Transition-Metal Dopants*, **Advanced Materials Interfaces**, 4, 1700579, (2017).
17. **J. Cheng**, J. Luo, and K. Yang, *Comparison Studies of Interfacial Electronic and Energetic Properties of LaAlO₃/TiO₂ and TiO₂/LaAlO₃ 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 MoS₂ 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 $A\text{HfO}_3/\text{SrTiO}_3$ ($A=\text{Ca}$, 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 $\text{LaAlO}_3/A^+\text{B}^{5+}\text{O}_3$* , **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 Catal.**, 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 $\text{LaAlO}_3/\text{SrTiO}_3$ 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 $\text{CaZrO}_3/\text{SrTiO}_3$ 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 $\text{LaAlO}_3/\text{SrTiO}_3$ 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*, **Journal of Chemical Physics**, 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 $\text{LaAlO}_3/\text{SrTiO}_3$ 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 $\text{AHfO}_3/\text{SrTiO}_3$ ($A = \text{Ca}, \text{Sr}, \text{and Ba}$) 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)