CHENG ZENG

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EDUCATION

Ph.D. in Chemical Engineering, Brown University — Sep 2017 - Aug 2022
Thesis title: Molecular Simulations by Exploiting Atomic Forces
Advisor: Andrew A. Peterson
Awards & Honors: Presidential fellow, Full member of Sigma Xi, Open graduate education program

M.Sc. in Data Science, Brown University — Sep 2019 - May 2022
Secondary master's degree outside the PhD program
Awards & Honors: Kaggle competition master (one gold and two silver medals)

B.Eng. and M.Eng. in Materials Science & Engineering, Tsinghua University — Sep 2009 - May 2016
Awards & Honors: National scholarship for encouragement, Beijing outstanding master's graduate

RESEARCH EXPERIENCE

Postdoctoral Research Fellow — Nov 2022 - Present
The Roux Institute — *Northeastern University, ME, USA*

- Led the research effort of design of high-entropy alloys for corrosion protection using an approach combining first-principles simulations and machine learning models.
- Led the development of a proposal titled "Understanding mechanics of brittle particle cold spray" for NSF Mechanics of Materials and Structures funding opportunity.
- Led the materials section for a collaborative proposal titled "Human-in-the-loop explainable AI design of high-entropy materials for the 21st century energy applications" for DOE Earthshot opportunities.
- Contributed literature review, public abstract and editing to a DOE Marine energy funding opportunity.

Graduate Research Assistant — Jan 2018 - Aug 2022
Catalyst Design Lab — *Brown University, RI, USA*

- Developed a nearsighted force training framework to systematically generate training data for large atomic structures. Implemented the approach in the atomistic machine learning package (AMP).
- Introduced force-based atomistic models to quantify the strain effect, surface relaxation and adsorbate-adsorbate interactions; Cut down atomistic simulations by 90%.
- Integrated machine learning models, a geometrical descriptor and a physical model to achieve all-site oxygen reduction activities for PtCo nanoparticles with sizes up to 17000 atoms. Quantified trends of size- and composition-dependencies on the oxygen reduction activity and stability. Explained many experimental observations.
- Established a machine learning assisted thermodynamic model to investigate the crossovers among different morphology of PtCo nanoparticles.
- Implemented machine learning accelerated genetic algorithms and Monte-Carlo simulations to find the most stable structure of PtCo nanoparticles. Discovered a new putative global minima. Introduced a new thermodynamic empirical model to explain the role of alloying element in crossover among various nanoparticle shapes.
- Constructed a surrogate machine learning model for global optimization of CO adsorbed on a Pt(111) surface with various coverages. Improved the simulation resolution by at least four fold.
- Conducted high throughput (>1800) electronic structure calculations in GPAW to establish the trends of strain effect for a variety of adsorption systems.
- Collaborated with experimental groups to screen oxygen reduction catalysts via a mechanic-based model. Identified a new ternary Pt alloy nanoparticle. Achieved a mass activity ∼31 times that of commercial Pt.
- Built a genetic algorithm to optimize initial neural network parameters to speed up training by 3x.

- Developed image/feature selection algorithms and neural network regularization to mitigate overfitting.

Research Assistant Sep 2016 - May 2017
Multiscale Simulation Group *State Nuclear Power Research Institute, Beijing, China*

- Conducted first-principles calculations in VASP to investigate hydrogen adsorption on transition metal doped zirconium (0001) surfaces.
- Studied the effect of an implicit water environment on the hydrogen adsorption.
- Employed a weighted d-band model to understand adsorption energy variations across various transition metals.
- Proposed a model based on electronegativity differences to explain solvation effects on adsorption.

Research Assistant Sep 2013 - May 2016
Lab of Advanced Materials *Tsinghua University, Beijing, China*

- Synthesized Cr doped alumina coatings on stainless steel surfaces by a cathodic micro arc deposition process. Identified the role of Cr doping on the phase transition to α type alumina.
- Prepared zirconia passive films on different types of zirconium alloys hydrothermally. Studied the role of tin and niobium doping on the hydrogen resistance of zirconia films. Proposed a point defect model to explain the roles of tin and niobium in modification of zirconium based passive films.
- Fabricated oxide films on stainless steel surfaces by *in situ* selective thermal oxidation. Optimized oxidation conditions for improved hydrogen resistance. Proposed a point defect model to understand the oxidation behavior at different temperatures.

PUBLICATIONS

1. **C. Zeng**, S.J. Sahoo, A.J. Medford & A.A. Peterson. The phase stability of large-size nanoparticle alloy catalysts at ab initio quality using a nearsighted force-training approach. arXiv preprint arXiv:2306.01846, 2023.
2. **Cheng Zeng**. Molecular Simulations by Exploiting Atomic Forces. Brown University, PhD dissertation, 2022.
3. **C. Zeng**†, T. A. Maark† & A. A. Peterson. Strain in catalysis: Rationalizing material, adsorbate, and site susceptibilities to biaxial lattice strain. The Journal of Physical Chemistry C 126(49), 20892-20902, 2022. († equal contributions)
4. **C. Zeng**, X. Chen & A. A. Peterson. A nearsighted force-training approach to systematically generate training data for the machine learning of large atomic structures. The Journal of Chemical Physics, 156(6), 064104, 2022.
5. J. Li, S. Sharma, K. Wei, Z. Chen, D., H. Lin, **Cheng Zeng** *et al.* Anisotropic strain tuning of $L1_0$ ternary nanoparticles for oxygen reduction. Journal of the American Chemical Society 142(45), 19209-19216, 2020.
6. S. Sharma, **C. Zeng** & A. A. Peterson. Face-centered tetragonal (FCT) Fe and Co alloys of Pt as catalysts for the oxygen reduction reaction (ORR): A DFT study. The Journal of Chemical Physics 15(4), 041704, 2019.
7. D. Yan, Q. Liu, **C. Zeng**, N. Dong, Y. Huang & W. Xiao. Adsorption of lithium polysulfides on an anatase (101) and an α-Al_2O_3 (0001) surface under an external electric field with first principles calculations. Applied Surface Science, 463, 331-338, 2019.
8. R. Tu, Q. Liu, **C. Zeng**, Y. Li, & W. Xiao. First principles study of point defect effects on iodine diffusion in zirconium. Nuclear Materials and Energy, 16, 238-244, 2018.
9. **C. Zeng**, B. Wang, L. Wang, Y. Li, Y. Nie, & W. Xiao. Chemisorption of a hydrogen adatom on metal doped α-Zr (0001) surfaces in a vacuum and an implicit solvation environment. Nuclear Materials and Energy, 13, 28-34, 2017.
10. **C. Zeng**, Y. Bai, L. Ling, Z. Xin, H. Liang, & X. Deng. Hydrogen interaction characteristics of nanoscale oxide films grown on iron-nickel based stainless steel by selective thermal oxidation. International Journal of Hydrogen Energy, 42(32), 20910-20921, 2017.
11. Z. Xin, Y. Ling, Y. Bai, **C. Zeng**, S. Wang, & J. Clara. Effect of hydrogen uptake on the electrochemical corrosion of N18 zircaloy under gamma irradiation. Applied Surface Science, 388, 252-258, 2016.

12. **C. Zeng**, Y. Ling, Y. Bai, W. Liu, & Y. Chen. Coupling effect of chromia doping and vacuum on the phase transition of alumina prepared by co-precipitation process. Powder Technology, 294, 284-291, 2016.
13. **C. Zeng**, Y. Ling, Y. Bai, R. Zhang, X. Dai, & Y. Chen. Hydrogen permeation characteristics of nanoscale passive films formed on different zirconium alloys. International Journal of Hydrogen Energy, 41(18), 7676-7690, 2016.
14. S. Wang, **C. Zeng**, Y. Ling, J. Wang, & G. Xu. Phase transformations and electrochemical characterizations of electrodeposited amorphous Fe-W coatings. Surface and Coatings Technology, 286, 36-41, 2016.
15. **C. Zeng**, Y. Ling, S. Li, Y. Rao, & Y. Chen. The effect of chromium on the gamma to alpha phase transition of alumina coating formed on 316L SS by a cathodic micro arc deposition (CMAD) process. Surface and Coatings Technology, 263, 15-20, 2015.

PRESENTATIONS

- Oral presentations

1. Machine learning accelerated design of corrosion-resistant high-entropy alloys. Academic Workshop at the Roux Institute, Northeastern University, June 2023.
2. Optimizing nanoparticle structures via neural-network-enhanced genetic algorithms and Monte-Carlo simulations. Academic Workshop at the Roux Institute, Northeastern University, Jan. 2023.
3. Molecular Simulations by Exploiting Atomic Forces. Seminar talk to The Williard Group of MIT, Virtually, Aug. 2022.
4. On-the-fly Machine Learning for Large Atomic Structures. Open Graduate Student Research Symposium, Brown University, Mar. 2022.
5. A Nearsighted Force-Training Approach for the Machine Learning of Large Atomic Structures. Winter Meeting of the New England Catalysis Society, Virtually, Feb. 2022.
6. Hydrogen permeation characteristics of nanoscale passive films formed on different zirconium alloys. NANOENERGY Conference, Manchester, UK, Jun. 2015.

- Poster presentations

1. First-principles and data-driven discovery of high-entropy alloys for corrosion protection. ICME 2023, Orlando, Florida, USA, May 2023.
2. Machine learning models with nearsighted force-training allow large-scale calculations at *ab initio* quality. Sigma Xi Student Research Conference, Virtually, Nov. 2021.
3. Hydrogen interaction characteristics of oxide films formed on stainless steel surfaces via selective oxidation. NANOENERGY Conference, Manchester, UK, Jun. 2015.

SKILLS

Simulation methods:	Machine learning, First-principles calculations, Molecular dynamics
Programming:	Python, BASH, C++, MATLAB, R, Julia, Fortran
Software management:	GitHub, Bitbucket, CI/CD, Unit testing
Database management:	MongoDB, MySQL

JOURNAL REVIEWER

- International Journal of Hydrogen Energy
- Surface and Coatings Technology
- Journal of Chemical Physics
- Applied Surface Science

- Journal of Materials Engineering and Performance

LEADERSHIP AND ACTIVITIES

- MOOC course instructor, "AI in Engineering" Lecture, Roux Institute, 2023
- Teaching Assistant, Chemical Engineering Thermodynamics, student feedback 4.92/5, Brown University, Fall 2021.
- Graduate student representative of recruitment fair for Brown University, AlChE annual meeting, 2021.
- Graduate peer mentor for international orientation, Brown University, 2021.
- Coordinator of biweekly project meetings among six research groups, Brown University, 2019 - 2020.
- Mentored and trained 1 postdoc, 1 graduate student and 2 undergraduate students, Brown University, 2018 - 2022.
- Vice president of graduate student union in School of Materials Science and Engineering, Tsinghua, 2015.