Richard Tran

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Department of Chemical Engineering
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Professional Development

- **University of Houston** 2023 - Present
  Postdoctoral Fellow - Chemical Engineering *Advisor: Lars Grabow*
- **Carnegie Mellon University** 2021 - 2023
  Postdoctoral Fellow - Chemical Engineering *Advisor: Zachary W. Ulissi*
- **University of California San Diego** 2016 - 2021
  Ph.D. - Nanoengineering (Materials Science focus) *Advisor: Shyue Ping Ong*
- **University of California San Diego** 2016 - 2017
  M.S. - Nanoengineering (Materials Science focus)
- **University of California San Diego** 2012 - 2015
  B.S. - Nanoengineering (Materials Science focus)

Digital Profiles

- Google Scholar
- LinkedIn
- Github

Skills and Competencies

- 9 years of professional experience in:
  - Academic research setting
  - Coding with Python
  - Software development and version control with Github and Git
  - Circle CI
  - AWS
  - Bash Scripting
  - High performance computing
  - Application of Vienna Ab initio Simulation Package (VASP) for density functional theory (DFT)
  - Application of related post-processing software:
    * Python Materials Genomics (pymatgen) (contributed to developments)
    * Atomic Simulation Environment (ASE)
    * Vaspkit (for wave-function analysis)
    * Bader analysis
    * LOBSTER for the analysis of Crystal Orbital Hamiltonian Populations
  - Scientific communication, including manuscript publication and conference presentation
  - High throughput workflow development for the full automation of DFT calculations
- 4 years of professional experience in applied machine learning in material and chemical engineering

Subject Expertise

- 9 years of applying computational methods in chemistry and material science
- 6 years investigating material science subjects
  - Structural materials: embrittlement of alloys through dopants, ceramic nanostructures for coating materials, investigation of grain boundaries
  - Surface science: surface thermodynamics, work function and electronic properties, nanoscale stability
  - Functional materials: Mott insulators and semiconductors, strongly correlated oxides
- 4 years investigating catalysts and catalytic reactions:
  - Bimetallic catalysts for NO_3^- reduction reaction
  - Oxide catalysts for oxygen evolution reaction
  - Multimetallic catalysts for liquid organic hydrogen carriers
  - Single atom catalysts for chlorine vs oxygen evolution selectivity

Research Experience

Post-Doctoral Fellow, Lars Grabow, University of Houston Dept of Chem. Eng. (2023-present)

- Applied high-throughput screening with machine learning to identify viable oxides for static and dynamic catalysis in the context of oxygen evolution reaction.
- Constructed automated high-throughput workflows for calculating the full reaction diagrams of single atom catalysts (doped graphene and MXenes) in the context of seawater electrolysis and chlorine evolution.
- Provided computational modelling for various investigations as part of the Center for Programmable Energy Catalysts.

Post-Doctoral Fellow, Zachary W. Ulissi, Carnegie Mellon University Dept of Chem. Eng. (2021-2023)

- Exploration of reaction diagrams and microkinetic models for the dehydrogenation of isopropyl alcohol using intermetallic catalyst surfaces.
- Developed software for the generalization of adsorbate placement on oxide surfaces for the application of oxygen evolution. Construction of machine learning models for the total DFT energies of adsorbed oxide surfaces.
- Screened the chemical space of binary intermetallics for potential candidates catalysts for nitrate reduction reaction using machine learning and previously developed microkinetic models.

Ph.D., Shyue Ping Ong, University of California San Diego Dept of NEng. (2016-2021)

- Developed high-throughput workflows for the calculation of surface properties of elemental crystalline solids.
- Explored dopant segregation at the grain boundaries and surfaces of refractory materials for the engineering of nanoscale structures.
- Investigation of defect induced metal-to-insulator transition in several Mott insulators for the application of neuromorphic computing.

Publications

1. R. Tran, L. Huang, Y. Zi, S. Wang, B. M. Comer, X. Wu, S. J. Raaijman, N. K. Sinha, S. Sadasivan, S. Thundiyil, K. B. Mamtani, G. Iyer, L. C. Grabow, L. Lu, and J. Chen, "Rational design of nanoscale stabilized oxide," *Nanoscale*, 2024 **(Corresponding)**
2. R. Tran, J. Lan, M. Shuaibi, B. M. Wood, S. Goyal, A. Das, J. Heras-Domingo, A. Kolluru, A. Rizvi, N. Shoghi, A. Sriram, F. Therrien, J. Abed, O. Voznyy, E. H. Sargent, Z. Ulissi, and C. L. Zitnick, "The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysts," *ACS Catalysis*, vol. 13, no. February, pp. 3066–3084, 2022
3. R. Tran, D. Wang, R. Kingsbury, A. Palizhati, K. A. Persson, A. Jain, and Z. W. Ulissi, "Screening of bimetallic electrocatalysts for water purification with machine learning," *The Journal of Chemical Physics*, vol. 157, no. 7, p. 074102, 2022
4. *T. Ren, R. Tran, S. Lee, A. Bandera, M. Herrera, X.-G. Li, S. P. Ong, and O. A. Graeve, "Morphology Control of Tantalum Carbide Nanoparticles through Dopant Additions," *The Journal of Physical Chemistry C*, vol. 125, no. 19, pp. 10665–10675, 2021

5. R. Tran, X. G. Li, S. P. Ong, Y. Kalcheim, and I. K. Schuller, "Metal-insulator transition in V2O3 with intrinsic defects," *Physical Review B*, vol. 103, no. 7, pp. 1–7, 2021

6. R. Tran, X.-G. Li, J. Montoya, D. Winston, K. A. Persson, and S. P. Ong, "Anisotropic work function of elemental crystals," *Surface Science*, vol. 687, no. September, pp. 48–55, 2019

7. R. Tran, Z. Xu, N. Zhou, B. Radhakrishnan, J. Luo, and S. P. Ong, "Computational study of metallic dopant segregation and embrittlement at molybdenum grain boundaries," in *Acta Materialia*, vol. 117, pp. 91–99, Elsevier Ltd, 2016

8. R. Tran, Z. Xu, B. Radhakrishnan, D. Winston, W. Sun, K. A. Persson, and S. P. Ong, "Surface energies of elemental crystals," *Scientific Data*, vol. 3, p. 160080, dec 2016

9. X. Wang, J. Musielewicz, R. Tran, S. Kumar Ethirajan, X. Fu, H. Mera, J. R. Kitchin, R. C. Kurchin, and Z. W. Ulissi, "Generalization of graph-based active learning relaxation strategies across materials," *Machine Learning: Science and Technology*, vol. 5, no. 2, pp. 0–9, 2024

10. S. Mondal, Z. Zhang, A. N. M. Na, R. Andrawis, S. Gamage, N. A. Aghamiri, Q. Wang, H. Zhou, F. Rodolakis, R. Tran, J. Kaur, C. Chen, S. P. Ong, A. Sengupta, Y. Abate, K. Roy, and S. Ramanathan, "All-Electric Nonassociative Learning in Nickel Oxide," *Advanced Intelligent Systems*, vol. 2200069, pp. 1–11, 2022

11. I. A. Zaluzhnyy, P. O. Sprau, R. Tran, Q. Wang, H. T. Zhang, Z. Zhang, T. J. Park, N. Hua, B. Stoychev, M. J. Cherukara, M. V. Holt, E. Nazaretski, X. Huang, H. Yan, A. Pattammattel, Y. S. Chu, S. P. Ong, S. Ramanathan, O. G. Shpyrko, and A. Frano, "Proton distribution visualization in perovskite nickelate devices utilizing nanofocused x rays," *Physical Review Materials*, vol. 5, no. 9, pp. 1–8, 2021

12. S. Cheng, M. H. Lee, R. Tran, Y. Shi, X. Li, H. Navarro, C. Adda, Q. Meng, L. Q. Chen, R. C. Dynes, S. P. Ong, I. K. Schuller, and Y. Zhu, "Inherent stochasticity during insulator-metal transition in VO2," *Proceedings of the National Academy of Sciences of the United States of America*, vol. 118, no. 37, 2021

13. M. J. Wahila, N. F. Quackenbush, J. T. Sadowski, J. O. Krisponeit, J. I. Flege, R. Tran, S. P. Ong, C. Schlueter, T. L. Lee, M. E. Holtz, D. A. Muller, H. Paik, D. G. Schlom, W. C. Lee, and L. F. Piper, "The breakdown of Mott physics at VO2 surfaces," *preprint submitted to arxiv*, pp. 1–9, 2020

14. H. Zheng, X. G. Li, R. Tran, C. Chen, M. Horton, D. Winston, K. A. Persson, and S. P. Ong, "Grain boundary properties of elemental metals," *Acta Materialia*, vol. 186, pp. 40–49, 2020

15. W. Wang, R. Tran, J. Qu, Y. Liu, C. Chen, M. Xu, Y. Chen, S. P. Ong, L. Wang, W. Zhou, and Z. Shao, "Chlorine-Doped Perovskite Oxide: A Platinum-Free Cathode for Dye-Sensitized Solar Cells," *ACS Applied Materials and Interfaces*, vol. 11, no. 39, pp. 35641–35652, 2019

16. M. F. V. Hidalgo, Y.-C. Lin, A. Grenier, D. Xiao, J. Rana, H. Xin, R. Tran, M. J. Zuba, J. Donohue, F. O. Omenya, I.-H. Chu, Z. Wang, X. Li, N. Chernova, K. W. Chapman, G. Zhou, L. F. Piper, S. P. Ong, and M. S. Whittingham, "Rational Synthesis and Electrochemical Performance of LiVOPO4 Polymorphs," *Journal of Materials Chemistry A*, vol. 7, no. 14, pp. 8423–8432, 2019

17. H. Zheng, R. Tran, X. G. Li, B. Radhakrishnan, and S. P. Ong, "Role of Zr in strengthening MoSi2 from density functional theory calculations," *Acta Materialia*, vol. 145, pp. 470–476, 2018

18. C. Chen, Z. Deng, R. Tran, H. Tang, I.-h. Chu, and S. P. Ong, "Accurate force field for molybdenum by machine learning large materials data," *Physical Review Materials*, vol. 043603, no. 1, pp. 1–10, 2017

*Co-first author

Manuscripts in preparation

1. R. Tran, M. Hilda, K.-E. You, J. Kitchin, and U. Zachary, "Rapid calculations of multimetallic reaction diagrams for isopropyl alcohol dehydrogenation,"

Proposals

- **ANL/CNM High Performance Computing Cluster (Carbon) Allocation (Awarded 512,000 CPU hours)**
  Effect of dopants on morphology of transition metal carbides, PI: Prof Shyue Ping Ong (2018)

- **Texas Center for Superconducting at UH (TcSUH) (Awarded $31,000 12 months)**
  Advancing the Hydrogen Economy while Decarbonizing the Chemical Industry through Chlorine-Mediated Electrocatalytic Synthesis, PI: Lars Grabow (2023)

- **UH Energy Transition Institute (ETI) Grant (Awarded $90,000 18 months)**
  Computational Prediction of Surface Stabilized Oxide Nanoparticles as High-Performance Oxygen Evolution Catalysts, PI: Prof Lars Grabow and Jiefu Chen (2024)

- **RAISE CET (Awarded $999,999)**
  Multidisciplinary High-Performance Computing and Artificial Intelligence Enabled Catalysis Design for Misco-Plasma Technologies in Clean Energy Transition, PI: Prof Lars Grabow and Jiefu Chen (2024)

- The Paul & Daisy Soros Fellowships for New Americans ($90,000 24 months)
  PI: Prof Shyue Ping Ong (2016 **Declined)**

- Molecular Sciences Software Institute ($50,000 12 months)
  Combinatorial defect engineering suite for heterogeneous catalysts, PI: Prof Zachary W. Ulissi (2021 **Declined)**

- DOE ERCAP
  Accelerating Catalyst Discovery with High-Throughput Calculations, Convolutional Networks, and Active Learning, PI: Zachary Ulissi (**Continuous)**

- Science Foundations for Energy Earthshot Allocation (512,000 hours)
  Catalyst Design for Micro-Plasma Assisted Hydrogen Generation, Long Duration Energy Storage, and Carbon Utilization, PI: Prof Jiefu Chen (2023 **Pending)**

- Global Centers Track 1.
  The Hydrogen Global Engineering Network (HydroGIN): An NSF/UKRI Global Research Center, PI: Prof Michael P. Harold (2023 **Pending)**

- DOD ONR (Laboratory equipment request)
  Artificial Intelligence Guided Self-Driving Laboratories for Autonomous Discovery of New Materials, **(Corresponding)** (2023 **Pending))**

Awards

- Pittsburgh Quantum Institute Uni-Pro Initiative for Conference Support
  Award amount of $1,500 for the Materials Research Society 2022

- University of Houston Postdoctoral Fellow Career and Travel Awards
  Award amount of $1,200 for the American Chemical Society 2024

Selected Presentations

- *An atomistic and continuum approach to dopant segregation and embrittlement at molybdenum grain boundaries.* Material Science and Technology, Salt Lake City, Utah, 2016.

- *The surface properties of elemental crystalline solids.* American Physical Society, Los Angeles, California, 2018.

- *Machine-learning assisted screening of catalytic materials.* **Invited**, Materials Research Society Spring Meeting and Exhibit, Honolulu, Hawaii, 2022.

Teaching and mentoring experience

- **Teaching assistant for Crystallography** Prof. Shyue Ping Ong, NanoEngineering, UCSD La Jolla, CA. 2018

- Mentored several graduate students and post-doctoral fellows in the group of Shyue Ping Ong, Zachary Ulissi, and Lars Grabow.

Digital Profiles

- Google Scholar

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- Github

Professional References

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