47 Olmsted Rd., Apt 216
Stanford, CA 94305
☎ +1 (773) 558 5371
✉ ctsai89@stanford.edu

Charlie Tsai

Education

2012–17 **Ph.D. in Chemical Engineering**, *Stanford University*, Stanford, CA, USA.
Additional coursework: Machine Learning, Convolutional Neural Networks, Databases

2012–14 **M.S. in Chemical Engineering**, *Stanford University*, Stanford, CA, USA.
GPA: 3.74

2008–12 **B.S. in Chemical Engineering**, *Northwestern University*, Evanston, IL, USA.
Minor in Philosophy, GPA: 3.9 (*magna cum laude*)

2010 **Exchange Student**, *Hong Kong University of Science and Technology*, Hong Kong.

Research Experience

2012– **Stanford University**, Adviser: Prof. Jens K. Nørskov.
Computational discovery of novel materials for energy transformation. Used density functional theory calculations to generate chemical data and develop models for predicting catalytic activity. Used Python for scripting and software development, along with R and SQL for data analysis. Initiated collaborations with five research groups, co-authored two successful grant proposals and 14+ publications.

2009–11 **Northwestern University**, Adviser: Prof. Joseph B. Lambert.
Used principal component and hierarchical clustering analysis (in SPSS) on nuclear magnetic resonance spectroscopy (NMR) data to distinguish and predict the geographical origins of fossilized resins (*e.g.* amber). Processed and analyzed hundreds of fossilized resin samples using NMR. (1 publication)

Additional Experience

2015 **Learning Chemical Trends in Heterogeneous Catalysis**, Stanford University.
Used supervise learning methods to predict catalytic activity for energy transformation processes using information from large chemical databases. Used Python with the scikit-learn package and SQL.

2015–16 **Teaching Assistant**, "Electronic Structure Theory", Stanford University.
Created problem sets, exams, and held weekly problem sessions. Designed a class-wide project for describing catalytic water dissociation using density functional theory, leading to a publication. Students used the Atomic Simulation Environment module in Python.

2015 **Molecular Dynamics Simulator**, Software Development Course Project, Stanford University.
Created a molecular dynamics simulator for modeling a gas using the Lennard-Jones potential with periodic boundary conditions. Written in C++ with a Python interface (via SWIG).

Computer Skills

Python (scikit-learn, numpy, SWIG, web.py), SQL, R, C++, MATLAB, UNIX, LaTeX

Honors & Awards

2013–16 National Science Foundation Graduate Research Fellowship

2012 AIChE Harry McCormack Outstanding Senior Student Award

2011 Initiative for Sustainability and Energy at Northwestern Summer Research Grant

2010 International Program Development Fellowship for International Study (HKUST)

2010 National Science Foundation REU Research Grant (Dartmouth College)

Languages

Native	English, Chinese (Mandarin)
Fluent	Chinese (Cantonese)
Beginning	Japanese, French

Selected Publications

Full list: `https://goo.gl/l6NqWR`

1. "Activating and Optimizing MoS_2 Basal Planes for Hydrogen Evolution Through the Formation of Strained Sulphur Vacancies", H. Li†, **C. Tsai**†, A. L. Koh, L. Cai, A. W. Contryman, A. H. Fragapane, J. Zhao, H. S. Han, H. C. Manoharan, F. Abild-Pedersen, J. K. Nørskov, and X. Zheng, *Nat. Mater.*, (2015), († equal contribution), (Top materials science and chemistry journal)
2. "Designing an Improved Transition Metal Phosphide Catalyst for Hydrogen Evolution using Experimental and Theoretical Trends", J. Kibsgaard, **C. Tsai**, K. Chan, J. D. Benck, J. K. Nørskov, F. Abild-Pedersen, and T. F. Jaramillo, *Energy Environ. Sci.*, 8, 3022–3029, (2015) (Top energy journal)
3. "Predicting Promoter-Induced Bond Activation on Solid Catalysts Using Elementary Bond Orders," **C. Tsai**, A. A. Latimer, J. S. Yoo, F. Studt, and F. Abild-Pedersen, *J. Phys. Chem. Lett*, 6, 3670–3674, (2015) (Top physical chemistry journal)
4. "Transition Metal Doped Edge Sites in Vertically Aligned MoS_2 Catalysts for Enhanced Hydrogen Evolution," H. Wang†, **C. Tsai**†, D. Kong, K. Chan, F. Abild-Pedersen, J. K. Nørskov, and Y. Cui, *Nano Res.*, 8 (2), 566–575 (2015). († equal contribution)
5. "Understanding the Reactivity of Layered Transition Metal Sulfides: A Single Electronic Descriptor for Structure and Adsorption," **C. Tsai**, K. Chan, J. K. Nørskov, and F. Abild-Pedersen, *J. Phys. Chem. Lett.*, 5, 3884–3889 (2014) (Top physical chemistry journal)
6. "Tuning the MoS_2 Edge-site Activity for Hydrogen Evolution *via* Support Interactions," **C. Tsai**, F. Abild-Pedersen, and J. K. Nørskov, *Nano Lett.* 14 (3), 1381–1387 (2014) (ESI Highly Cited Paper)
7. "Distinguishing Amber and Copal Classes by Proton Magnetic Resonance Spectroscopy," J. B. Lambert, **C. Y.-H. Tsai**, M. C. Shah, A. E. Hurtley, A. E., and J. A. Santiago-Blay, *Archaeometry* 54 (2), 332–348 (2012)