Charlie Tsai

Curriculum Vitae

Department of Chemical Engineering
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Education

- 2017 **Ph.D. in Chemical Engineering**, Stanford University, Stanford, CA, USA.
- (expected) Advisor: Jens K. Nørskov
 - 2014 M.S. in Chemical Engineering, Stanford University, Stanford, CA, USA.
 - 2012 **B.S. in Chemical Engineering**, *Northwestern University*, Evanston, IL, USA. Minor in Philosophy
 - 2010 Exchange Student, Hong Kong University of Science and Technology, Hong Kong.

Experience

- 2012 **Prof. Jens K. Nørskov**, *Stanford University*, Stanford, CA, USA.
- Present Used density functional theory to develop concepts for understanding and designing catalytic materials for a variety of processes in energy conversion.
- 2010 2012 **Prof. Kimberly A. Gray**, *Northwestern University*, Evanston, IL, USA. Synthesized ${\rm TiO_2}$ nanorods and nanotubes with selectively exposed facets for photocatalytic ${\rm CO_2}$ reduction. Used transmission electron microscopy (TEM) and X-ray diffraction (XRD) for characterization.
- 2009 2010 **Prof. Joseph B. Lambert**, *Northwestern University*, Evanston, IL, USA.

 Used principal component and hierarchical clustering analysis on nuclear magnetic resonance spectroscopy (NMR) data to distinguish and predict the geographical origins of fossilized resins.

Honors & Awards

- 2013 National Science Foundation Graduate Research Fellowship
- 2012 AIChE Harry McCormack Outstanding Senior Award
- 2011 Initiative for Sustainability and Energy at Northwestern Summer Research Grant
- 2010 International Program Development Fellowship for International Study at HKUST
- 2010 National Science Foundation REU Grant in Nanomaterials at Dartmouth College
- 2010 Tau Beta Pi Engineering Honor Society
- 2010 Omega Chi Epsilon Chemical Engineering Honor Society
- 2010 AIChE Donald F. Othmer Academic Excellence Award

Publications

- Total (First author): 17 (9)
- 17. "Evaluating the Structural Dependence of Predicted Reaction Rates in Catalytic Water Dissociation," C. Tsai, K. Lee, A. J. Medford, H. Aljama, L. D. Chen, C. F. Dickens, T. S. Geisler, C. J. Guido, T. M. Joseph, C. S. Kirk, A. A. Latimer, X. Liu, B. Loong, R. J. McCartey, J. H. Montoya, L. Power, A. R. Singh, J. J. Willis, M. M. Winterkorn, M. Yuan, J. Wilcox, J. K. Nørskov, (2015), in preparation
- 16. "Scaling Relationships for Binding Energies on Transition Metal Complexes," Y. Wang, J. H. Montoya, C. Tsai, M. S. G. Alquist, J. K. Nørskov, F. Studt, (2015), in preparation
- 15. "Chemical and Phase Evolution of Amorphous Molybdenum Sulfide Catalysts for Electrochemical Hydrogen Production Directly Observed Using Environmental Transmission Electron Microscopy," S. Lee, J. Benck, C. Tsai, J. Park, F. Abild-Pedersen, T. F. Jaramillo, R. Sinclair, (2015), in preparation
- 14. "Activating and Optimizing the MoS₂ Basal Plane for Hydrogen Evolution using Strained Sulfur 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), *accepted*
- "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.*, (2015)
- 12. "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*, (2015)
- 11. "The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations," J. H. Montoya, C. Tsai, A. Vojvodic, and J. K. Nørskov, *ChemSusChem*, 8 (13), 2180-2186 (2015)
- "Theoretical Insights into the Hydrogen Evolution Activity of Layered Transition Metal Dichalcogenides," C. Tsai, K. Chan, J. K. Nørskov, and F. Abild-Pedersen, Surf. Sci, 640, 133–140, (2015)
- "Transition Metal Doped Edge Sites in Vertically Aligned MoS₂ 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)
- 8. "Rational Design of MoS₂ Catalysts: Tuning the Structure and Activity *via* Transition Metal Doping," **C. Tsai**, K. Chan, J. K. Nørskov, and F. Abild-Pedersen, *Catal. Sci. Technol.*, 5, 246–253 (2015)

- 7. "Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst During the Hydrogen Evolution Reaction," H. G. Sanchez Casalongue, J. D. Benck, **C. Tsai**, S. Kaya, M. L. Ng, F. Abild-Pedersen, J. K. Nørskov, H. Ogasawara, T. F. Jaramillo, and A. Nilsson, *J. Phys. Chem. C*, 118 (50), 29252–29259 (2014)
- 6. "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)
- "Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO₂ reduction," K. Chan, C. Tsai, H. Hansen, J. K. Nørskov, ChemCatChem, 6 (7), 1899–1905 (2014)
- 4. "Active Edge Sites in MoSe₂ and WSe₂ Catalysts for the Hydrogen Evolution Reaction: A Density Functional Study," **C. Tsai**, K. Chan, F. Abild-Pedersen, and J. K. Nørskov, *Phys. Chem. Chem. Phys.*, 16, 13156–13164 (2014)
- 3. "Tuning the MoS₂ 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**)
- 2. "Synthesis of High-energy Anatase Nanorods *via* an Intermediate Nanotube Morphology," D. Finkelstein-Shapiro, C. Y.-H. Tsai, S. Li, and K. A., Gray, *Chem. Phys. Lett.* 546, 106–108 (2012)
- 1. "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)

Conference Presentations

- 3. ECAT 2014 Symposium (Whistler, BC, Canada), "Rational Design of MoS₂ Catalysts by Transition Metal Doping" (poster), (2014)
- 2. Pacific Coast Catalysis Society Meeting (Stanford, CA, USA), "Tailoring the Structure and Activity of MoS₂ Catalysts by Transition Metal Doping" (poster), (2014)
- 1. AIChE Annual Meeting (San Franciso, CA, USA), "Support Interactions in MoS₂ for Hydrogen Evolution" (oral presentation), (2013)

Computer Skills

Python (including SWIG), C++, R, MATLAB/Octave, Mathematica, LATEX, Microsoft Excel, Adobe Illustrator, Cinema 4D

Languages

English Native

Chinese Native (Mandarin) and fluent (Cantonese)

Japanese Beginning

French Beginning