

Bin Liu

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EDUCATION

- 2008 **Colorado School of Mines**, Golden, CO
Ph.D. in Chemical Engineering
Advisors: Prof. James Ely and Prof. Mark Lusk
- 2003 **Dalian University of Technology**, Dalian, China
B.S. in Chemical Engineering

PROFESSIONAL EXPERIENCE

- Kansas State University**, Department of Chemical Engineering, Manhattan, KS
- *Assistant Professor*, 08/2013 – present
- Carnegie Mellon University**, Department of Chemical Engineering, Pittsburgh, PA
- *Postdoctoral research associate*, 01/2013 – 07/2013
Supervisor: Prof. John R. Kitchin
- Argonne National Laboratory**, Center for Nanoscale Materials, Argonne, IL
- *Postdoctoral research associate*, 01/2010 – 12/2012
Supervisor: Dr. Jeffrey Greeley
- Colorado School of Mines**, Department of Chemical Engineering, Golden, CO
- *Postdoctoral research associate*, 01/2009 – 12/2010
Supervisor: Prof. Anthony M. Dean
- California Institute of Technology**, Materials and Process Simulation Center, Pasadena, CA
- *Visiting student*, 01/2005 – 04/2005
Supervisors: Prof. William A. Goddard III and Dr. Adri van Duin (now Prof. at Penn State)

HONORS AND AWARDS

- KSU Faculty Mentoring Fellowship, 2014
- Academic Excellence Award, 2015
- KSU Faculty Development Award, 2016
- College of Engineering Outstanding Tenure-track Assistant Professor Award, 2016

COURSES TAUGHT

- CHE 735 Chemical Engineering Analysis I – Fall 2013, Fall 2015
- CHE 320 Chemical Process Analysis – Spring 2014, Spring 2015, Spring 2016

REFEREED JOURNALS

1. Zhou, M., Le, T.N.-M., Huyhn, L.K., Liu, B., "Effects of Structure and Size of Ni Nanocatalysts on Hydrogen Selectivity via Water-Gas-Shift Reaction - A First-Principles-Based Kinetic Study", (*Under review*).
2. Zeng, F., Tenn, W.J. III, Aki, A.N.V.K., Xu, J., Liu, Bin, Hohn, K.L., "Influence of basicity on 1, 3-butadiene formation from catalytic 2, 3-butanediol dehydration over γ -alumina", (*Under review*).

3. Tang, J., Liu, B. "Reactivity of Hematite (α -Fe₂O₃) (0001) Surface for Methane Oxidation: A GGA + U Study ", Journal of Physical Chemistry C, **2016**, 120, 12, 6642-6650.
4. Zhou, M., Liu, B. "A DFT Investigation on the Selectivity of Water-Gas Shift Reaction on Clean and Potassium Modified Ni(111) Surface", ChemCatChem, **2015**, 7, 23, 3928-3935.
5. Liu, B., Zhou, M., Chan, M.K.Y., Greeley, J.P., "Understanding Polyol Decomposition on Bimetallic Pt-Mo Catalysts - A DFT Study of Glycerol", ACS Catalysis, **2015**, 5, 8, 4942-4950.
6. Gu, X., Liu, B., Greeley, J.P., "First-Principles Study of Structure Sensitivity of Ethylene Glycol Conversion on Platinum", ACS Catalysis, **2015**, 5, 4, 2623-2631.
7. Lei, Y., Liu, B., Lu, J., Lin, X., Gao, L., Guisinger, N.P., Greeley, J.P., Elam, J.W., "Synthesis of palladium nanoparticles on TiO₂(110) using a beta-diketonate precursor", Physical Chemistry Chemical Physics, **2015**, 17, 9, 6470-6477.
8. Detwiler, M.D., Gharachorlou, A., Mayr, L., Gu, X.-K., Liu, B., and Greeley, J., Delgass, W.N., Ribeiro, F.H., and Zemlyanov, D.Y., "Reaction of trimethylaluminum with water on Pt(111) and Pd(111) from 10⁻⁵ to 10⁻¹ millibar", Journal of Physical Chemistry C, **2015**, 119, 2399-2411.
9. Lu, J., Liu, B., Greeley, J.P., Guisinger, N.P., Stair, P.C., and Elam, J.W., "First-principles predictions and in situ experimental atomic layer deposition on metal surfaces", Chemistry of Materials, **2014**, 26, 6752-6761.
10. Lei, Y., Liu, B., Lu, J., Libera, J. A., Greeley, J. P., and Elam, J. W., "Effects of chlorine in titanium oxide on palladium atomic layer deposition", Journal of Physical Chemistry C, **2014**, 118, 22611-22619.
11. Nguyen, M. L. T., Liu, B., and Huynh, L. K., "SurfKin - An ab initio kinetic code for modeling surface reactions", Journal of Computational Chemistry, **2014**, 35, 1890-1899.
12. Lei, Y., Zhao, H., Rivas, R. D., Lee, S., Liu, B, Lu, J., Stach, E. S., Winans, R. E., Chapman, K. W., Greeley, J. P., Miller, J. T., Chupas, P. J., and Elam, J. W., "Adsorbate-induced structural changes in 1-3 nm platinum nanoparticles", Journal of the American Chemical Society, **2014**, 136, 9320-9326.
13. Liu, B., Cheng, L., Curtiss, L., and Greeley, J.P., "Effects of van der Waals density functional calculations on trends in furfural adsorption and hydrogenation on close-packed transition metal surfaces", Surface Science **2014**, 622, 51-59.
14. Cheng, L., Yin, C., Mehmood, F., Liu, B., Greeley, J., Lee, S., Lee, B., Seifert, S., Winans, R., Teschner, D., Schloegl, R., Vajda, S., and Curtiss, L. "Reaction mechanism for direct propylene epoxidation by alumina-supported silver aggregates: The role of the particle/support interface", ACS Catalysis, **2014** 4, 1, 32-39.
15. Liu, B. and Greeley, J.P., "A DFT-based analysis of trends in glycerol decomposition on close-packed transition metal surfaces", Physical Chemistry Chemical Physics, **2013**, 15, 6475-6485
16. Lei, Y., Lu, J., Zhao, H., Liu, B., Low, K.-B., Wu, T., Libera, J.A., Greeley, J.P., Chupas, P.J., Miller, J.T. and Elam, J.W., "Resolving Deligation of Palladium (II) beta-Diketonate

- and Nucleation of Palladium Nanoparticles Synthesized by Atomic Layer Deposition”. *Journal of Physical Chemistry C*, **2013** 117, 11141-11148.
17. Knoll, A., Lau, K.C., Chan, M.K.Y., Liu, B., Greeley, J.P., Curtiss, L., Hereld, M. and Papka, M.E. “Uncertainty classification and visualization of molecular surfaces”, *International Journal for Uncertainty Quantification*, **2013**, 3(2), 157-169.
 18. Liu, B. and Greeley, J.P. “Density functional theory study of C-O bond scission and selectivity considerations in glycerol decomposition on Pt(111)”, *Topics in Catalysis*, **2012**, 55, 280-289.
 19. Lei, Y., Liu, B., Lu, J., Lobo, R., Wu, T., Feng, H., Xia, X., Mane, A.U., Libera, J.A., Greeley, J.P., Miller, J.T. and Elam, J.W., “Synthesis of Pt-Pd core-shell nanostructures by atomic layer deposition: Application in propane oxidative dehydrogenation to propylene”, *Chemistry of Materials*, **2012**, 24, 3525-3533.
 20. Lu, J., Liu, B., Greeley, J.P., Feng, Z., Joseph A. Libera, J.A., Lei, Y., Bedzyk, M.J., Stair, P.C., and Elam, J.W., “Protective porous alumina growth on palladium nanoparticles by self-poisoned atomic layer deposition”, *Chemistry of Materials*, **2012**, 24, 2047-2055.
 21. Liu, B., Lusk, M.T., and Ely, J.F. “Reactive molecular dynamics simulations of hydrocarbon dissociation on Ni(111) surfaces”, *Surfaces Science*, **2012**, 606, 615-623.
 22. Liu, B., and Greeley, J.P. “Decomposition pathways of glycerol via C-H, O-H and C-C bond scission on Pt(111): A density functional theory study”, *Journal of Physical Chemistry C*, **2011**, 115, 19702-19709.
 23. Liu, B., Lusk, M.T and Ely, J.F. “The influence of nickel catalyst geometry on the dissociation barriers of H₂ and CH₄: Ni₁₃ vs. Ni(111)”, *Journal of Physical Chemistry C*, **2009**, 113, 13715-13722.
 24. Liu, B., Lusk, M.T. and Ely, J.F. “Hydrogen dissociations on small nickel clusters”, *Molecular Simulation*, **2009**, 35(10), 928-935.
 25. Liu, B., Lusk, M.T., Ely, J.F., van Duin; A.C.T., and Goddard, W.A. III “Reactive molecular dynamics force field for the dissociation of light hydrocarbons on Ni(111)”, *Molecular Simulation*, **2008**, 34(10-15), 967-972.