

Department of Chemical and Biomolecular Engineering  
240D McCourtney Hall  
University of Notre Dame  
Notre Dame, IN 46556

E-mail: [cobrie23@nd.edu](mailto:cobrie23@nd.edu)  
Phone: (574) 631-5706

## PROFESSIONAL EMPLOYMENT

2017-present Assistant Professor, Department of Chemical and Biomolecular Engineering,  
University of Notre Dame, Notre Dame, IN

2014-2017 Postdoctoral Fellow, Sensors and Electron Devices Directorate, U.S. Army  
Research Laboratory, Adelphi, MD

2011-2014 Postdoctoral Fellow, Chemical Physics Department, Fritz Haber Institute of the  
Max Planck Society, Berlin, Germany

## EDUCATION

Ph.D. Chemical Engineering, Carnegie Mellon University, 2011

B.S. Chemical Engineering, University of Colorado at Boulder, 2006

## PUBLICATIONS

### Peer Reviewed Journal Articles

23. **C.P. O'Brien**, I.C. Lee, "The Interaction of CO with PdCu Alloy Hydrogen Separation Membranes: An Operando Infrared Spectroscopy Study," *Catal. Today*, in press.
22. K.-H. Dostert, **C.P. O'Brien**, F. Mirabella, F. Ivars-Barcelo, S. Attia, E. Spadafora, S. Schauermaun, H.-J. Freund, "Selective Partial Hydrogenation of Acrolein on Pd: A Mechanistic Study," *ACS Catalysis* 7 (2017) 5523-5533.

21. **C.P. O'Brien**, I.C. Lee, "CO Poisoning and CO Hydrogenation on the Surface of Pd Hydrogen Separation Membranes," *J. Phys. Chem. C.* 121 (2017) 16864-16871.
20. W. Liu, Y. Jiang, K.-H. Dostert, **C.P. O'Brien**, W. Riedel, A. Savara, S. Schaueremann, A. Tkatchenko, "Catalysis beyond frontier molecular orbitals: Selectivity in partial hydrogenation of multi-unsaturated hydrocarbons on metal catalysts," *Sci. Adv.* 3 (2017) e1700939.
19. **C.P. O'Brien**, I.C. Lee, "Kinetic Modeling of Spillover and Temperature-Programmed Oxidation of Oxy-Carbon Surface Species on Pt/Al<sub>2</sub>O<sub>3</sub>," *J. Phys. Chem. C.* 121 (2017) 12329-12336.
18. **C.P. O'Brien**, I.C. Lee, "A detailed spectroscopic analysis of the growth of oxy-carbon species on the surface of Pt/Al<sub>2</sub>O<sub>3</sub> during propane oxidation," *J. Catal.* 347 (2017) 1-8.
17. **C.P. O'Brien**, Z. W. Dunbar, I.C. Lee, "A spectroscopic membrane permeation cell for *in-situ* infrared-reflection absorption spectroscopic analysis of membrane surfaces and simultaneous measurement of trans-membrane gas permeation rates," *J. Membr. Sci.* 526 (2017) 43-51.
16. **C.P. O'Brien**, K.-H. Dostert, S. Schaueremann, H.-J. Freund, "Selective Hydrogenation of Acrolein over Pd Model Catalysts: Temperature and Particle-Size Effects," *Chem. Eur. J.* 22 (2016) 15856-15863.
15. **C. O'Brien**, K.-H. Dostert, M. Hollerer, C. Stiehler, F. Calaza, S. Schaueremann, S. Shaikhutdinov, M. Sterrer, H.-J. Freund, "Supports and Modified Nano-particles for Designing Model Catalysts," *Faraday Discuss.* 188 (2016) 309-321.
14. K.-H. Dostert, **C.P. O'Brien**, F. Mirabella, F. Ivars-Barcelo, S. Schaueremann, "Adsorption of Acrolein, Propanal, and Allyl Alcohol on Pd(111): A Combination of Infrared Reflection-Absorption Spectroscopy and Temperature-Programmed Desorption Studies," *Phys. Chem. Chem. Phys.* 18 (2016) 13960-13973.
13. K.-H. Dostert, **C.P. O'Brien**, W. Liu, W. Riedel, A. Savara, A. Tkatchenko, S. Schaueremann, H.-J. Freund, "Adsorption of isophorone and trimethyl-cyclohexanone on Pd(111): A combination of infrared reflection absorption spectroscopy and density functional theory calculations," *Surf. Sci.* 650 (2016) 149-160.

12. **C.P. O'Brien**, G.R. Jenness, H. Dong, D.G. Vlachos, I.C. Lee, "Deactivation of Pt/Al<sub>2</sub>O<sub>3</sub> during propane oxidation at low temperatures: Kinetic regimes and platinum oxide formation," *J. Catal.* 337 (2016) 122-132.
11. P. Dementyev, K.-H. Dostert, F. Ivars-Barcelo, **C.P. O'Brien**, F. Mirabella, S. Schauermaun, X. Li, J. Paier, J. Sauer, H.-J. Freund, "Water Interaction with Iron Oxides," *Angew. Chem. Int. Ed.* 54 (2015) 13942-13946.
10. K.-H. Dostert, **C.P. O'Brien**, F. Ivars-Barcelo, S. Schauermaun, H.-J. Freund, "Spectators Control Selectivity in Surface Chemistry: Acrolein Partial Hydrogenation over Pd," *J. Am. Chem. Soc.* 137 (2015) 13496-13502.
9. K.-H. Dostert, **C.P. O'Brien**, W. Riedel, A. Savara, W. Liu, M. Oehzelt, A. Tkatchenko, S. Schauermaun, "Interaction of Isophorone with Pd(111): A Combination of IRAS, NEXAFS, and DFT Studies," *J. Phys. Chem. C* 118 (2014) 27833-27842.
8. M. Peter, J.M.F. Camacho, S. Adamovski, **C.P. O'Brien**, K.-H. Dostert, S. Schauermaun, H.-J. Freund, "Trends in the binding strength of surface species on nanoparticles: how does the adsorption energy scale with the particle size," *Angew. Chem. Int. Ed.* 52 (2013) 5175-5179.
7. **C.P. O'Brien**, J.B. Miller, B.D. Morreale, A.J. Gellman, "H<sub>2</sub>-D<sub>2</sub> exchange kinetics in the presence of H<sub>2</sub>S over Pd<sub>4</sub>S, Pd<sub>70</sub>Cu<sub>30</sub>, and Pd<sub>47</sub>Cu<sub>53</sub> surfaces," *J. Phys. Chem. C* 116 (2012) 17657-17667.
6. **C.P. O'Brien**, J.B. Miller, B.D. Morreale, A.J. Gellman, "The kinetics of H<sub>2</sub>-D<sub>2</sub> exchange over Pd, Cu, and PdCu foil surfaces," *J. Phys. Chem. C* 115 (2011) 24221-24230.
5. **C.P. O'Brien**, J.B. Miller, A.J. Gellman, B.D. Morreale, "The hydrogen permeability of Pd<sub>4</sub>S," *J. Membr. Sci.* 371 (2011) 263-267.
4. **C.P. O'Brien**, B.H. Howard, J.B. Miller, B.D. Morreale, A.J. Gellman, "Inhibition of hydrogen transport through Pd and Pd<sub>47</sub>Cu<sub>53</sub> membranes by H<sub>2</sub>S at 350 °C," *J. Membr. Sci.* 349 (2010) 380-384.
3. J.B. Miller, D.R. Alfonso, B.H. Howard, **C.P. O'Brien**, B.D. Morreale, "Hydrogen dissociation on Pd<sub>4</sub>S surfaces," *J. Phys. Chem. C* 113 (2009) 18800-18806.

2. N.B. Cramer, **C.P. O'Brien**, C.N. Bowman, "Mechanisms, polymerization rate scaling, and oxygen inhibition with an ultra-rapid monovinyl urethane acrylate," *Polymer* 49 (2008) 4756-4761.
1. J.A. Carioscia, L. Schneidewind, **C. O'Brien**, R. Ely, C. Feeser, N. Cramer, C.N. Bowman, "Thiol-norbornene materials: Approaches to develop high T<sub>g</sub> thiol-ene polymers," *J. Polym. Sci., Part A: Polym. Chem.* 45 (2007) 5686-5696.

### **In Submission**

H. Kareem, S. Shan, F. Lin, J. Li, B. Prasai, **C. O'Brien**, I. Lee, D. Tran, L. Yang, D. Mott, J. Luo, V. Petkov, C.-J. Zhong, "HE-XRD/PDF Characterization and in-situ DRIFTS probing of Composition-Tunable Synergy of Gold-Palladium Nanoalloys for Catalytic Oxidation of Carbon Monoxide," *Cat. Sci. Tech.*

### **Invention Disclosures**

**C.P. O'Brien**, I.C. Lee, Z. W. Dunbar, "A spectroscopic membrane permeation cell for *in-situ* infrared-reflection absorption spectroscopy and simultaneous gas permeation measurements," U.S. Army Research Laboratory Invention Disclosure ARL 16-38 (2016).

### **AWARDS AND HONORS**

- 2016 Outstanding Post-doctoral Student Poster, Gordon Research Conference on Catalysis
- 2014 U.S. Army Research Laboratory Postdoctoral Fellowship
- 2010 Ph.D. Student Presentation Prize, Pittsburgh-Cleveland Catalysis Society Meeting

### **INVITED TALKS**

- 2017 "Rational Catalyst Design from Model Studies with a Molecular-beam/Surface-spectroscopy Apparatus," Oregon State University, Department of Chemical, Biological and Environmental Engineering, Corvallis, OR (March 17).
- 2017 "Rational Catalyst Design from Model Studies with a Molecular-beam/Surface-spectroscopy Apparatus," University of Notre Dame, Department of Chemical and Biomolecular Engineering, Notre Dame, IN (March 2).

- 2016 "Deactivation of Pt/Al<sub>2</sub>O<sub>3</sub> during Propane Combustion at Low Temperatures," University of Arizona, Tucson, AZ (April 26).
- 2016 "Deactivation of Pt/Al<sub>2</sub>O<sub>3</sub> during Propane Combustion at Low Temperatures," University of Central Florida, Orlando, FL (April 4).
- 2015 "Spectators Govern Selective Surface Chemistry: Acrolein Partial Hydrogenation over Pd." Lawrence Berkeley National Laboratory, Berkeley, CA (March 17).
- 2015 "Spectators Govern Selective Surface Chemistry: Acrolein Partial Hydrogenation over Pd." BASF Catalysts, Iselin, NJ (March 16).
- 2014 "Selective Hydrogenation of Acrolein over Pd Model Catalysts," U.S. Army Research Laboratory, Adelphi, MD (April 9).
- 2011 "Sulfur Poisoning of Pd and PdCu Alloy Hydrogen Separation Membranes," Fritz Haber Institute of the Max Planck Society, Berlin, Germany (February 14).
- 2011 "Sulfur Poisoning of Pd and PdCu Alloy Hydrogen Separation Membranes," University of Illinois at Chicago (January 26).

## **CONFERENCE ACTIVITY**

### **Oral Presentations**

- 2017 "Operando membrane spectroscopy: A novel technique for identifying membrane structure-function relationships," ACS National Meeting, San Francisco, CA (April 2-6).
- 2017 "Quantitative spectroscopic analysis of the role of oxy-carbon surface species in the mechanism of propane oxidation over Pt/Al<sub>2</sub>O<sub>3</sub>," ACS National Meeting, San Francisco, CA (April 2-6).
- 2016 "Formation of platinum oxide films on the surface of platinum nanoparticles during propane oxidation," ACS National Meeting, Philadelphia, PA (August 21-25).

- 2015 "The role of surface species in propane oxidation over Pt/Al<sub>2</sub>O<sub>3</sub>," ACS National Meeting, Denver, CO (March 22-27).
- 2010 "The kinetics of H<sub>2</sub>-D<sub>2</sub> exchange over Pd, Cu, and PdCu foil surfaces," AIChE, Salt Lake City, UT (November 7-12).
- 2010 "Surface alloys for control of sulfur corrosion in Pd-based H<sub>2</sub> separation membranes" Pittsburgh-Cleveland Catalysis Society Meeting, Pittsburgh, PA, (May 14).
- 2010 "Surface alloys for control of sulfur corrosion in Pd-based H<sub>2</sub> separation membranes," ACS National Meeting, San Francisco, CA (March 21-25).
- 2009 "Development of sulfur tolerant hydrogen separation membranes," International Pittsburgh Coal Conference, Pittsburgh, PA (September 20-23).
- 2009 "Inhibition of hydrogen transport through Pd and Pd<sub>47</sub>Cu<sub>53</sub> membranes by H<sub>2</sub>S," Pittsburgh-Cleveland Catalysis Society Meeting, Pittsburgh, PA (May 29).
- 2008 "Sulfur tolerant coatings for dense metal hydrogen separation membranes," Pittsburgh-Cleveland Catalysis Society Meeting, State College, PA (June 9).

### Posters

- 2016 "Formation of platinum oxide films on the surface of platinum nanoparticles during propane combustion," Gordon Research Conference on Catalysis, New London, NH (June 12-17).
- 2015 "The influence of sulfur on carbon deposition on Pt/Al<sub>2</sub>O<sub>3</sub> catalysts during alkane oxidation," North American Catalysis Society Meeting, Pittsburgh, PA (June 14-19).
- 2013 "Chemoselective Hydrogenation of Acrolein over Pd Model Catalysts," EuropaCat XI, Lyon, France (September 1-6).
- 2012 "Particle Size Dependent Hydrogenation of Acrolein over Pd/Fe<sub>3</sub>O<sub>4</sub> Model Catalysts," ECOS-29, Edinburgh, Scotland (September 2-7).
- 2012 "Adsorption of Isophorone on Pd(111) and Pd/Fe<sub>3</sub>O<sub>4</sub>: Temperature Programmed Desorption and IRAS Studies," IWOX VIII, Baqueira de Beret, Spain (January 15-20).

2008 "Sulfur tolerant hydrogen separation membranes," ChEGSA Research Symposium, Pittsburgh, PA (October).