

DEAN R. WHEELER

Department of Chemical Engineering
Brigham Young University, Provo, UT 84602

PROFESSION PREPARATION

University of California, Berkeley	<i>Ph.D. Chemical Engineering, 2002</i> Thesis: "Molecular simulations of diffusion in electrolytes" Professor John S. Newman, Advisor
Brigham Young University Provo, Utah	<i>B.S. Chemical Engineering, magna cum laude, 1996</i> <i>Minor in Arabic</i>

RESEARCH AND EDUCATIONAL APPOINTMENTS

- *Assistant Professor* (2003-present), Chemical Engineering, Brigham Young University, Provo, Utah
- *Graduate Research Assistant and Graduate Student Instructor* (1997-2002), Lawrence Berkeley National Lab and University of California, Berkeley
- *Educational Director for Nonprofit Organization* (1996-1997), AMIDEAST Foundation, Amman, Jordan
- *Semester Research Appointment* (1994), Brookhaven National Lab, under the direction of Senior Scientist Radoslav Adzic
- *Summer Research Program* (1994), MIT Biotechnology Process Engineering Center, under the direction of Professor Linda Cima

AWARDS

- NSF Faculty Early Career Development Award (2006-2011)
- Daniel Cubicciotti Student Award of the Electrochemical Society (2002)
- NSF Graduate Fellowship (1997-2000)
- Presidential Scholar, Brigham Young University (1989-1996)

RESEARCH FOCUS

Molecular Electrochemistry. Developing experimental tools and computer models to understand and control molecular processes in electrochemical systems. Current applications include lithium batteries, fuel cells, and electrodeposition.

RESEARCH FUNDING

- J. Harb (PI), R. Davis, M. Linford, D. Wheeler, and A. Wooley, “NIRT: Chemically Directed Surface Alignment and Wiring of Self-Assembled Nanoelectrical Circuits,” National Science Foundation, \$1M, 7/01/07 to 6/31/11.
- D. Wheeler (PI), “CAREER: Design of large-scale molecular simulations of electrocatalysis,” National Science Foundation, \$400k, 2/01/06 - 1/31/11.
- D. Wheeler (PI) and J. Harb, “Design, optimization, and fabrication of high-performance electrodes for the next generation of Li-ion batteries,” U.S. Dept. of Energy BATT Program, \$579k, 9/01/04 - 8/31/08.
- D. Wheeler (PI), “Novel molecular simulations for understanding the function of additives in electrodeposition,” American Chemical Society – PRF, \$35k, 3/01/05 - 8/31/07.
- J. Harb (PI), D. Wheeler, and M. Linford, “SGER: Exploratory methods for nanowire fabrication on insulating substrates,” National Science Foundation, \$100k, 3/15/05 - 3/31/07
- J. Harb (PI) and Dean Wheeler, “Fundamental investigation of mixed-oxide cathodes for rapid-charge lithium-ion batteries,” Office of Naval Research, \$75k, 9/01/05 - 8/31/06

PEER-REVIEWED PUBLICATIONS

- C.L. Guymon, J.N. Harb, R.L. Rowley, and D.R. Wheeler, “MPSA effects on copper electrodeposition investigated by molecular dynamics simulations,” *J. Chem. Phys.*, in press (2007).
- D.E. Stephenson, E.M. Hartman, J.N. Harb, and D.R. Wheeler, “Modeling of particle-particle interactions in porous cathodes for lithium-ion batteries,” *J. Electrochem. Soc.* **154**, A1146-A1155 (2007).
- M. Linford, M. Lee, K. Nelson, L. Hutchins, H. Becerril, S. Cosby, J. Blood, D. Wheeler, R. Davis, A. Woolley, and J. Harb, “Nanografting of silanes on silicon dioxide with applications to DNA localization and copper electroless deposition,” *Chem. Mater.* **19**, 5052-5054 (2007).
- M. Tan, C. Guymon, D.R. Wheeler, and J.N. Harb, “The role of SPS, MPSA, and chloride in additive systems for copper electrodeposition,” *J. Electrochem. Soc.* **154**, D78-D81 (2007).
- I. Thorat, V. Mathur, J. Harb, and D. Wheeler, “Performance of carbon-fiber-containing LiFePO₄ cathodes for high-power applications,” *J. Power Sources* **162**, 673-678 (2006).
- D. Wheeler, “A simple classroom demonstration of natural convection,” *Chem. Eng. Educ.* **39**, 138-141 (2005).
- C. Guymon, R. Rowley, J. Harb, and D. Wheeler, “Simulating an electrochemical interface using charge dynamics,” *Cond. Matt. Phys.* **8**, 335-356 (2005).
- H. Becerril, R. Stoltenberg, D. Wheeler, R. Davis, J. Harb, and A. Woolley, “DNA-templated three-branched nanostructures for nanoelectronic devices,” *J. Amer. Chem. Soc.* **127**, 2828-2829 (2005).
- D. Wheeler and J. Newman, “Molecular dynamics simulations of multicomponent

diffusion: 2. Nonequilibrium method,” *J. Phys. Chem. B* **108**, 18362-18367 (2004).

- D. Wheeler and J. Newman, “Molecular dynamics simulations of multicomponent diffusion: 1. Equilibrium method,” *J. Phys. Chem. B* **108**, 18353-18361 (2004).
- J. Newman, K. Thomas, D. Wheeler, and H. Hafezi, “Modeling of lithium-ion batteries,” *J. Power Sources* **119**, 838-843 (2003).
- D. Wheeler and J. Newman, “A less expensive Ewald lattice sum,” *Chem. Phys. Lett.* **366**, 537-543 (2002).
- D. Wheeler and R. Rowley, “Shear viscosity of polar liquid mixtures via non-equilibrium molecular dynamics: water, methanol, and acetone,” *Molec. Phys.* **94**, 555-564 (1998).
- D. Wheeler, N. Fuller, and R. Rowley, “Non-equilibrium molecular dynamics simulation of the shear viscosity of liquid methanol: Adaptation of the Ewald sum to Lees-Edwards boundary conditions,” *Molec. Phys.* **92**, 55-62 (1997).
- D. Wheeler, J. Wang, and R. Adzic, “The effects of anions on the underpotential deposition of Tl on Pt(111): A voltammetric study,” *J. Electroanal. Chem.* **387**, 115-119 (1995).

PRESENTATIONS AT INTERNATIONAL CONFERENCES

- I. Thorat, D. Stephenson, V. Mathur, B. Walker, E. Hartman, J. Harb, and D. Wheeler, “Effect of morphology and thickness on high-rate discharge performance of porous composite cathodes,” 212th Meeting of the Electrochemical Society, Washington, DC, 2007.
- D. Wheeler and C. Guymon, “Simulating the electrochemical double layer using charge dynamics,” 2006 Annual Meeting of AIChE, San Francisco, CA.
- D. Stephenson, I. Thorat, E. Hartman, J. Harb, and D. Wheeler, “Fundamental investigation of inter-particle contact in porous composite cathodes,” 210th Meeting of the Electrochemical Society, Cancun, Mexico, 2006.
- D. Stephenson, D. Wheeler, and J. Harb, “Fundamental investigation of mixed-oxide cathodes for rapid-charge lithium-ion batteries,” 209th Meeting of the Electrochemical Society, Denver, CO, 2006.
- K. Nelson, J. Blood, S. Cosby, M. Lee, J. Harb, D. Wheeler, M. Linford, A. Woolley and R. Davis, “Selective metallization of AFM-patterned functionalized silane monolayers,” 208th Meeting of the Electrochemical Society, Los Angeles, CA, 2005.
- C. Guymon, J. Harb and D. Wheeler, “MPSA behavior near a copper surface through molecular simulation and experiment,” 208th Meeting of the Electrochemical Society, Los Angeles, CA, 2005.
- V. Mathur, I. Thorat, D. Wheeler and J. Harb, “Carbon-fiber containing LiFePO₄ cathodes for high-power applications,” 208th Meeting of the Electrochemical Society, Los Angeles, CA, 2005.
- C. Guymon and D. Wheeler, “Simulated additive behavior in a copper-deposition bath using molecular dynamics,” 206th Meeting of the Electrochemical Society, Honolulu, HI, 2004.

- D. Wheeler, G. Gessel, A. Henrichsen, and M. Winters, "Molecular simulations of lithium and anion transport in liquid carbonate electrolytes," 206th Meeting of the Electrochemical Society, Honolulu, HI, 2004.
- D. Wheeler, "A better Ewald lattice sum," 2002 Annual Meeting of AIChE, Indianapolis, IN.
- D. Wheeler and J. Newman, "Molecular dynamics simulations of diffusion in lithium battery electrolytes," 2001 Annual Meeting of AIChE, Reno, NV.
- D. Wheeler and J. Newman, "Molecular dynamics simulations of multicomponent diffusion in liquid electrolytes," 196th Meeting of the Electrochemical Society, Honolulu, HI, 1999.
- D. Wheeler and R. Rowley, "Non-equilibrium molecular dynamics of liquid mixture shear viscosity," 1997 Annual Meeting of AIChE, Los Angeles, CA.
- H. Huang, D. Wheeler, and G. Watt, "Ligand reactivity of Femoco isolated from the nitrogenase enzyme," Abstr. Amer. Chem. Soc. 208, 495-INOR (1994).

INVITED PRESENTATIONS

- D. Wheeler and P. Balbuena, "Modeling of low-temperature fuel cells," NSF Workshop on Low-Temperature Fuel Cells, Arlington, VA, 2005.
- D. Wheeler, "Simulating the electrochemical interface using charge dynamics," Symposium on Basic and Applied Statistical Physics of Condensed Matter (in Honor of the 70th Birthday of Douglas Henderson), Provo, UT, 2004.
- D. Wheeler, "The engineering of water rockets," Brigham Young University, Chemical Engineering Department, 2003.
- D. Wheeler, "The technology of lithium batteries and fuel cells," University of Nevada at Reno, Chemical Engineering Department, 2003.
- D. Wheeler, "Molecular simulations of diffusion in electrolytes," University of Nevada at Reno, Chemical Engineering Department, 2003.
- D. Wheeler, "Molecular simulations of diffusion in electrolytes," University of California, Berkeley, Chemical Engineering Department, 2002.
- D. Wheeler, "Molecular dynamics simulations of aqueous electrolytes," Meeting of the San Francisco Section of The Electrochemical Society, 2000.

GRADUATE STUDENTS ADVISED

- Clint Guymon, Ph.D. (2003 - 2005)
- Mark Winters, M.S. (2003 - 2006)
- David Stephenson, M.S. (2004 - present)
- Indrajeet Thorat, Ph.D. (2004 - present)
- Abhishek Asthana, Ph.D. (2005 - present)
- Dane Hansen, Ph.D. (2006 - present)
- Elliott Bird, M.S. (2007 - present)