Ryan Jorn

Assitant Professor of Chemistry
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RESEARCH INTERESTS:

- Mesoscale electron and ion transport theory/simulation
- Chemistry and energy transfer at surfaces
- Electrochemical energy storage and energy conversion
- Method development for scattering theory
- Molecular machines and molecular electronics
- Vibrational relaxation and dissipative processes

EDUCATION:

Northwestern University - Evanston,IL **2003-2009**
Ph.D. Chemistry
Thesis Advisor: Tamar Seideman
Thesis Title: Inelastic Rate Processes in Molecular Junctions:
Current-induced Nuclear Excitation and
Bath-induced Vibrational Decoherence

Ripon College - Ripon,WI **1999-2003**
B.A. Chemistry, B.A. Physics
summa cum laude
Senior Thesis Title: An Investigation of Thermally Induced Crazing
in BC-408 Scintillating Plastic

RESEARCH EXPERIENCE:

Villanova University - Villanova, PA **2013-Present**
Assistant Professor of Chemistry

A research program at Villanova is being built that is focused on modeling electrochemical interfaces utilizing novel computational approaches. Work is already underway to develop a new computational method for describing charge transfer processes in molecular dynamics simulations by combining electron scattering theory with software written for the LAMMPS package. Additional projects include modeling ion diffusion from the electrolyte into surface films in lithium-ion batteries and new theoretical developments for describing electron scattering at interfaces.

Argonne National Laboratory - Argonne, IL **2010-2013**
Postdoctoral Researcher - CELS Division

Research involved multi-scale modeling of both materials and interfaces relevant to fuel cell and energy storage technologies. As a result of this work, an important connection was made between continuum mechanics, coarse-grained molecular dynamics, and atomistic simulations of proton transport through polymer membranes. In addition, the graphite/electrolyte interface in lithium-ion batteries was investigated and the effect of applied bias voltages and surface films was elucidated.

Northwestern University - Evanston,IL **2003-2010**
Graduate Research Assistant & Postdoctoral Researcher

Research involved deriving new theoretical models to describe electron scattering in the context of molecular electronics. A new approach was developed based on ensemble-scattering to describe coherent excitation of nuclear degrees of freedom during charge transport combined with dissipative vibrational dynamics. Non-equilibrium Green's function calculations were used to parameterize the electron-phonon interactions and collaborations were pursued to study several examples of current-induced dynamics.

HONORS AND AWARDS:

Northwestern University

Donald E. Smith Teaching Award	2006
Phi Lambda Epsilon Honorary Chemical Society	2005

Ripon College

Phi Beta Kappa Honor Society	2003
Eka Francian Chemistry Honor Society	2002
William Barber Award in Physics	2002
Leone Oyster '19 Memorial Scholarship in Chemistry	2002
Clifford Krump Phi Beta Kappa Award	2001
Franklin L. Stone Award In Chemistry	2001
Larry Barker 1940 Award in Chemistry	2000
Pickard Scholarship – Awarded to Promising Freshman	1999

PUBLICATIONS:

1. S. R. G. Kankanamge, K. Li, K. D. Fulfer, P. Du, R. Jorn, R. Kumar, D. G. Kuroda. *Mechanism behind the Unusually High Conductivities of High Concentrated Sodium Ion Glyme-Based Electrolytes.*,J. Phys. Chem. C. **2018**, *122* (44) 25237-25246.

2. L. Raguette and R. Jorn. *Ion Solvation and Dynamics at Solid Electrolyte Interphases: A Long Way from Bulk?*,J. Phys. Chem. C. **2018**, *122* (6), 3219-3232.

3. K. Li, S. R. G. Kankanamge, T. K. Weldeghiorghis, R. Jorn, D. G. Kuroda, and R. Kumar.*Predicting Ion Association in Sodium Electrolytes: A Transferrable Model for Investigating Glymes*,J. Phys. Chem. C. **2018**, *122* (9), 4747-4756.(**awarded cover of issue**)

4. R. Jorn and R. Kumar. *Breaking the Scales: Electrolyte Modeling in Metal-Ion Batteries*,Elec. Soc. Interface **2017**, *26* (1), 55-59.

5. J. Wahlers, K. D. Fulfer, D. P. Harding, D. G. Kuroda, R. Kumar, and R. Jorn. *Solvation Structure and Concentration in Glyme-Based Sodium Electrolytes: A Combined Spectroscopic and Computational Study*,J. Phys. Chem. C. **2016**, *120* (32), 17949-17959.

6. R. Jorn, R. Kumar, D. Abraham, G.A. Voth. *Atomistic Modeling of the Electrode-Electrolyte Interface in Li-ion Energy Storage Systems: Electrolyte Structuring*,J. Phys. Chem. C. **2013**, *117* (8), 3747-3761.

7. R. Jorn, J. Savage, and G.A. Voth. *Proton Conduction in Exchange Membranes Across Multiple Length Scales*, Acc. Chem. Res. **2012**, *45* (11), 2002-2010.

8. R. Jorn, and G.A. Voth. *Mesoscale Simulation of Proton Transport in Proton Exchange Membranes*, J. Phys. Chem. C **2012**, *116*, 10476. (**awarded cover of issue**)

9. R. Jorn, J. Zhao, H. Petek, and T. Seideman. *Current-Driven Dynamics in Molecular Junctions: Endohedral Fullerenes*, ACS Nano **2011**,*5*, 7858.

10. G.E. Lindberg, C. Knight, R. Jorn, J.F. Darma, and G.A. Voth. *Multiscale Simulation of Hydroxide Solvation and Transport in Anion Exchange Membranes*, ECS Trans. **2011**, *41*, 1785.

11. H. Sarode, M.A. Vandiver, A.M. Maes, B. Caire, J.L. Horan, Y. Yan, Y. Li, G.E. Lindberg, J.F. Darma, C. Knight, R. Jorn, M.E. Lenz, R. Kasper, S. Gu, B. Zhang. *Designing Alkaline Exchange Membranes from Scratch*,ECS Trans. **2011**, *41*, 1761.

12. N. Yoder, R. Jorn, M.C. Hersam, and T. Seideman. *Current-Driven Desorption at the Organic Molecule-Semiconductor Interface: Cyclopentene on Si(100)*, publication in *Current-Driven Phenomena in Nanoelectronics*, (World Scientific **2011**).

13. R. Jorn and T. Seideman. *Implications and Applications of Current-Induced Dynamics in Molecular Junctions*, Acc. Chem. Res. **2010**, *43* 1186.

14. R. Jorn and T. Seideman. *Competition Between Current-Induced Excitation and Bath-Induced Decoherence in Molecular Junctions*, J. Chem. Phys. **2009**, *131* 244114.

15. R. Jorn. and T. Seideman. *Dissipation in Molecular Junctions*, J. Chem. Phys. **2008**, *129*, 194703.

16. R. Jorn, E. Livshits, R. Baer, and T. Seideman. *The Role of Charge Localization in Current-Driven Dynamics*, Israel J. Chem. **2007**, *47*, 99.

17. N.L. Yoder, N.P. Guisinger, M.C. Hersam, R. Jorn, C.-C. Kaun, and T. Seideman. *Saturated Hydrocarbons on Silicon: Quantifying Desorption with Scanning Tunneling Microscopy and Quantum Theory* Phys. Rev. Lett. **2006**, *2*, 0607621.

18. C.-C. Kaun, R. Jorn, and T. Seideman. *Spontaneous Oscillation of Current in Fullerene Molecular Junctions* Phys. Rev. B **2006**, *74*, 045415.

19. R. Jorn and T. Seideman. *Theory of Current Induced Dynamics in Molecular-Scale Devices* J. Chem. Phys. **2006**, *124*, 084703.

PRESENTATIONS:

1. *Middle Atlantic Regional Meeting of the American Chemical Soceity*, **Invited Talk**: "From Molecular Electronics to Energy Storage: Striving for a Unified Approach to Electron Transfer in Open Systems", Hershey, PA, June 2017.

2. *Haverford College Chemistry Seminar*, **Invited Talk**: "Advancing Energy Storage from iPhones to F-150's: Computational Investigation of Solvation Structure in Metal-Ion Batteries", Haverford, PA, October 2016.

3. *252nd American Chemical Society National Meeting*, **Contributed Talk**: "Electron Scattering in Liouville Space: From coherence to decoherence to incoherence?", Philadelphia, PA, August 2016.

4. *Louisiana State University Physical Chemistry Seminar*, **Invited Talk**: "Tackling Multi-Scale Challenges of Batteries from the Atom Up", Baton Rouge, LA, September 2015.

5. *American Physical Society Meeting*, **Invited Talk**: "Multiscale Modeling of Proton Transport in Fuel Cell Membranes", Boston, MA, March 2012.

6. *Computational Molecular Science Mini-Symposium - University of Chicago*, **Invited Talk**: "Mesoscale Modeling of Proton Transport in Fuel Cell Membranes", Chicago, IL, September 2011.

7. *219th Electrochemical Society Meeting*, **Contributed Talk**: "Mesoscale Modeling of Ion Transport: Application to Polyelectrolyte Membranes", Montreal, Canada, May 2011.

8. *38th Midwest Theoretical Chemistry Conference*, **Contributed Talk**: "Theory of Current Induced Dynamics in Molecular Junctions.", The Ohio State University, June 2006.

TEACHING EXPERIENCE:

Assistant Professor - CHEM 1151 Gen. Chem. Lecture **2016 - Present**
Villanova University - Villanova, PA

Assistant Professor - CHEM 9447 Comp. Chemistry **2015 - Present**
Villanova University - Villanova, PA

Assistant Professor - CHEM 3412 Quantum Chemistry **2014 - Present**
Villanova University - Villanova, PA

Assistant Professor - CHEM 1103 Gen. Chem. Lab. **2013 - Present**
Villanova University - Villanova, PA

Assistant Professor - CHEM 3403 PChem Thermo. Lab. **2013 - Present**
Villanova University - Villanova, PA

Adjunct Professor - Phys 114 College Physics I Lab. **2012**
Benedictine University - Lisle, IL

OTHER SKILLS:

- German- Intermediate reading, writing, and verbal skills
- FORTRAN, Bash shell scripting,C++
- Windows, Linux, Unix
- MPI parallel programming
- Q-chem, GAMESS, Microsoft Office, LaTex,LAMMPS,CP2K