

## Matt K. Petersen, Ph.D.

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Center for Integrated Nano Technologies  
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### Education

2006: Ph.D. Physical Chemistry, University of Utah

*Proton transport and solvation in complex environments.* Gregory A. Voth, Chair

2000: B.S. Mathematics, Physics minor, University of Idaho

1998: B.S. Professional Chemistry, University of Idaho

### Recent Positions

2007-Current: Post-Doctoral Fellow,

Center for Integrated Nano Technologies, Sandia National Labs

2006: Post-Doctoral Fellow,

Department of Chemistry and Center for Biophysical Modeling and Simulation, University of Utah

### Select Publications

Petersen, Matt K.; Hatt, Alison J.; Voth, Gregory A. **Orientational Dynamics of Water in the Nafion Polymer Electrolyte Membrane and Its Relationship to Proton Transport.** *Journal of Physical Chemistry B* (2008), 112(26), 7754-7761.

Petersen, Matt K.; Voth, Gregory A. **Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion.** *Journal of Physical Chemistry B* (2006), 110(37), 18594-18600.

Petersen, Matt K.; Voth, Gregory A. **Amphiphilic Character of the Hydrated Proton in Methanol-Water Solutions.** *Journal of Physical Chemistry B* (2006), 110(14), 7085-7089.

Petersen, Matt K.; Wang, Feng; Blake, Nick P.; Metiu, Horia; Voth, Gregory A. **Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion.** *Journal of Physical Chemistry B* (2005), 109(9), 3727-3730.

Lapid, Hadas; Agmon, Noam; Petersen, Matt K.; Voth, Gregory A. **A bond-order analysis of the mechanism for hydrated proton mobility in liquid water.** *Journal of Chemical Physics* (2005), 122(1), 14506.

Petersen, Matt K.; Iyengar, Srinivasan S.; Day, Tyler J. F.; Voth, Gregory A. **The Hydrated Proton at the Water Liquid/Vapor Interface.** *Journal of Physical Chemistry B* (2004), 108(39), 14804-14806.

## **Relevant Skills**

### ***Methods***

Molecular Dynamics, Non-equilibrium Molecular Dynamics, Monte Carlo, Extended Ensemble MC (i.e. parallel tempering), Electronic Structure, QM/MM, experienced with force-field development and method development/implementation.

### ***Codes***

LAMMPS (C++ MD simulator), DL POLY (Fortran MD simulator), DL EVB and SCI DL EVB (Fortran/C reactive potential MD simulator), Gaussian/Gauss View, VMD (analysis/molecular visualization).

### ***Programming***

Experienced with Fortran, C++, Linux/UNIX shell scripting.

### ***OS/Computers***

Experienced with Linux/UNIX, BSD/OSX, Windows. Familiar with various message passing implementations, i.e. Open MPI, MPICH, MVAPICH, SGI-MPT, and their use ranging from large scale supercomputer clusters to multi-processor desktops. Experienced with PBS and LSF batch scripting.

### ***Leadership/Teamwork***

As a graduate student I led a portion of my advisor's group focusing on topics in proton transport. This six-ten member group considered problems ranging from enzymatic catalysis and transmembrane proton transport to proton conduction in polyelectrolyte membranes.

## **Research Positions**

2007-Current: Post-Doctoral Fellow,  
Center for Integrated Nano Technologies, Sandia National Labs

2006: Post-Doctoral Fellow,  
Department of Chemistry and Center for Biophysical Modeling and Simulation, University of Utah

2004-2006: Research Assistant,  
Department of Chemistry and Center for Biophysical Modeling and Simulation, University of Utah

2002-2004: Research Assistant,  
Department of Chemistry and Henry Eyring Center for Theoretical Chemistry,  
University of Utah

2001: Henry Eyring Fellow,  
Henry Eyring Center for Theoretical Chemistry, University of Utah

1999-2000: Research Assistant,  
Ecological and Conservation Genetics Laboratory, University of Idaho

1999: Research Assistant,  
Hyperfine Interactions Laboratory, University of Washington

1998: Research Assistant,  
Resonance Raman spectroscopy for the study of electron transfer, University of Idaho

## **Recent Talks**

### ***Invited***

#### **Shear Rheology Through Computer Simulation.**

Corning Incorporated; Corning, New York (8/2008)

#### **Improving Proton Transport Membranes: Lessons From Molecular Dynamics.**

Eastern Washington University; Cheney, Washington (3/2007)

#### **Explicit Proton Transport and Solvation in Simple Fluids and Hydrated Nafion.**

Center for Integrated Nano Technology, Sandia National Laboratories-New Mexico; Albuquerque, New Mexico (1/2007 )

### ***Conference***

#### **Shear Thinning in Nanoparticle Suspensions.**

APS March 2008; New Orleans, Louisiana (3/2008)

#### **Effect of Nanoparticle Shape and Size on Shear Rheology.**

APS March 2008; New Orleans, Louisiana (3/2008)

#### **Proton Transport Coupling to Solvent Rearrangements in the Perfluorosulfonic Acid Membrane Nafion.**

ECS spring 2007; Chicago, Illinois (5/2007)

#### **Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion.**

AIChE 2006 Annual Meeting; San Fransisco, California (11/2006)

## **Teaching Positions**

2001-2002: Teaching Assistant,  
Department of Chemistry, University of Utah

1997-1999: Teaching Assistant,  
Department of Chemistry, University of Idaho

## **Professional Memberships**

The American Physical Society  
The Electrochemical Society  
American Institute of Chemical Engineers

## **Awards/Fellowships**

Henry Eyring Fellowship,  
Henry Eyring Center for Theoretical Chemistry, University of Utah

## **All Publications**

in 't Veld, Pieter; Petersen, M. K.; Grest, G.S. **Shear Thinning of Nanoparticle Suspensions.** Physical Review E (2009), 79(2), 021401.

Brown, W. M.; Petersen, M. K.; Plimpton, S. J.; Grest, G.S. **Liquid Crystal Nanodroplets in Solution.** Journal of Chemical Physics (2009), 130(4), 044901.

Petersen, Matt K.; Hatt, Alison J.; Voth, Gregory A. **Orientational Dynamics of Water in the Nafion Polymer Electrolyte Membrane and Its Relationship to Proton Transport.** Journal of Physical Chemistry B (2008), 112(26), 7754-7761.

Swanson, Jessica M. J.; Maupin, C. Mark; Chen, Hanning; Petersen, Matt K.; Xu, Jiancong.; Wu, Yujie.; Voth, Gregory A. **Proton Solvation and Transport in Aqueous and Biomolecular Systems: Insights from Computer Simulations.** Journal of Physical Chemistry B (2007), 111(17), 4300-4314 (feature article).

Petersen, Matt K.; Voth, Gregory A. **Characterization of the Solvation and Transport of the Hydrated Proton in the Perfluorosulfonic Acid Membrane Nafion.** Journal of Physical Chemistry B (2006), 110(37), 18594-18600.

Petersen, Matt K.; Voth, Gregory A. **Amphiphilic Character of the Hydrated Proton in Methanol-Water Solutions.** Journal of Physical Chemistry B (2006), 110(14), 7085-7089.

Burnham, Christian J.; Petersen, Matt K.; Day, Tyler J. F.; Iyengar, Srinivasan S.; Voth, Gregory A. **The properties of ion-water clusters. II. Solvation structures of Na<sup>+</sup>, Cl<sup>-</sup>, and H<sup>+</sup> clusters as a function of temperature.** Journal of Chemical Physics (2006), 124(2), 024327

Petersen, Matt K.; Wang, Feng; Blake, Nick P.; Metiu, Horia; Voth, Gregory A. **Excess Proton Solvation and Delocalization in a Hydrophilic Pocket of the Proton Conducting Polymer Membrane Nafion.** Journal of Physical Chemistry B (2005), 109(9), 3727-3730.

Lapid, Hadas; Agmon, Noam; Petersen, Matt K.; Voth, Gregory A. **A bond-order analysis of the mechanism for hydrated proton mobility in liquid water.** Journal of Chemical Physics (2005), 122(1), 14506.

Iyengar, Srinivasan S.; Petersen, Matt K.; Day, Tyler J. F.; Burnham, Christian J.; Teige, Virginia E.; Voth, Gregory A. **The properties of ion-water clusters. I. The protonated 21-water cluster.** Journal of Chemical Physics (2005), 123(8), 084309.

Blake, Nick P.; Petersen, Matt K.; Voth, Gregory A.; Metiu, Horia. **Structure of Hydrated Na-Nafion Polymer Membranes.** Journal of Physical Chemistry B (2005), 109(51), 24244-24253.

Petersen, Matt K.; Iyengar, Srinivasan S.; Day, Tyler J. F.; Voth, Gregory A. **The Hydrated Proton at the Water Liquid/Vapor Interface.** Journal of Physical Chemistry B (2004), 108(39), 14804-14806.

Iyengar, Srinivasan S.; Burnham, Christian J.; Petersen, Matt K.; Voth, Gregory A. **Modeling condensed-phase chemistry through molecular dynamics simulation.** Computing in Science & Engineering (2003), 5(4), 31-35.