

# Maria Demireva

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**SUMMARY:** Strong background in physical chemistry and mass spectrometry. Extensive experience using experimental gas phase techniques (e.g., IR and UV photodissociation spectroscopy, collisional activation, electron capture dissociation), and theoretical methods (e.g., electronic structure calculations, molecular dynamics, master equation) to investigate the structures, energetics, and kinetics of various complexes and reactions. Ability to successfully plan, execute, and communicate research ideas and results, as demonstrated by a considerable publication and presentation record. Conceived and submitted ideas for project proposals that were accepted by outside groups as part of collaborations. Hard working, fast learner, curious, motivated, and enthusiastic about science.

**EDUCATION:** **University of Utah, Salt Lake City (2014 – Dec. 2017)**  
Ph.D. in (Physical) Chemistry (Defended Dec. 2017, Degree Conferred May 2018)  
Ph.D. Dissertation: “*Thermochemistry and Reactivity of Gadolinium Cation ( $Gd^+$ ): Energetics and Mechanistic Insights for Reactions with Hydrogen, Its Isotopologues, and Various Oxides*”  
GPA: 4.0

**University of North Carolina, Chapel Hill (2003 – 2007)**  
B.S. Chemistry with Distinction and Honors - GPA: 3.5  
Minor: Mathematics - GPA: 3.7  
Lund University, Sweden, study abroad, Spring 2005

## RESEARCH EXPERIENCE:

- ◆ **Post-graduate research, University of Utah, Prof. Peter B. Armentrout, Jan. 2018 – present.**
  - Investigate the effect of protonation site on the energetics and fragmentation of the test molecule p-aminobenzoic acid using guided ion beam tandem mass spectrometry and theory.
  - Study reactions of the lanthanide samarium cation ( $Sm^+$ ) with hydrogen and its isotopologues.
  
- ◆ **Graduate research, University of Utah, Prof. Peter B. Armentrout, 2014 – Dec. 2017.**
  - Used guided ion beam tandem mass spectrometry to investigate the activation of small neutrals (including  $O_2$ ,  $CO_2$ , and  $H_2$ ) by the lanthanide gadolinium cation ( $Gd^+$ ).
  - Measured first direct experimental 0 K bond energies for  $GdO^+$ ,  $GdC^+$ ,  $GdCO^+$ ,  $GdH^+$ ,  $Gd^+-O_2$ ,  $OGd^+-O$ ,  $Gd^+-OCO$ , and  $OGd^+-CO$ .
  - Experimentally mapped the potential energy surfaces for the activation of  $O_2$  and  $CO_2$  by  $Gd^+$ .
  - Performed extensive electronic structure calculations for comparison with the experimental thermochemistry and for insight into the reaction mechanisms.
  - Elucidated periodic trends from comparisons of  $Gd^+$  reactivity with other metal cations.
  
- ◆ **Graduate research, UC Berkeley, 2007 – 2013.**
  - Used Fourier transform ion cyclotron resonance mass spectrometry in combination with various ion activation methods (collisions with neutrals, electron capture, absorption of IR or UV photons) and theoretical calculations to:
    - Characterize the interactions, dissociation kinetics, and energetics of non-covalently bound gas-phase systems.

- Study ion solvation and its effect on ion structure and reactivity of isolated hydrated ion clusters in the gas phase.
- Measure relative and absolute one-electron reduction potentials of ions whose potentials are difficult to measure with traditional solution-phase electrochemistry methods.
- Wrote software to numerically solve a master equation for investigating the energetics and kinetics of blackbody absorption and dissociation of molecules and clusters. Used my software in collaboration with Prof. Travis Fridgen's group (Memorial University of Newfoundland) to model their data from blackbody infrared radiative dissociation experiments to:
  - Determine the bond energies of  $\text{Ca}^{2+}$  bound uracil clusters.
  - Characterize the interaction strengths of halogen binding anion receptors.
- **FOM (The Netherlands), Prof. Jos Oomens, Oct. 30<sup>th</sup> – Nov. 10<sup>th</sup>, 2011.**  
Investigated the role of anion size and degree of methylation on halide anion binding to diprotonated diamino-compounds with infrared multiple photon dissociation spectroscopy using a free electron laser.
- **EPFL (Switzerland), Prof. Thomas R. Rizzo, Nov. 11<sup>th</sup> – Dec. 2<sup>nd</sup>, 2011.**  
Used cryogenic ion infrared-ultraviolet spectroscopy to investigate the effect of bond dissociation energies on radical migration in peptides.
- ◆ **Undergraduate research, UNC Chapel Hill, Prof. Gary L. Glish, 2006 – 2007.**  
Investigated collisional relaxation rates as a function of bath-gas pressure for different sized peptide ions in ion trap mass spectrometry.

#### TEACHING EXPERIENCE:

- ◆ **Graduate student instructor, UC Berkeley:**
  - Fall 2008 and 2009, analytical chemistry laboratory.
  - Fall 2007, general chemistry laboratory.
- ◆ **Teaching assistant, UNC Chapel Hill:**
  - Summer 2006, analytical chemistry laboratory.
- ◆ **Professor's aid for grading, UNC Chapel Hill:**
  - Spring 2007, introductory differential equation mathematics course.

#### AWARDS:

- ◆ **Cheves T. Walling Graduate Research Award (University of Utah, 2018).** Given for the most outstanding Chemistry Ph.D. dissertation.
- ◆ **Richard A. Schaeffer Memorial Fund Travel Award for ASMS 2013.**

#### SKILLS:

- ◆ **Theoretical methods:**
  - Master equation to model ion internal energy distributions resulting from blackbody dissociation (wrote program).
  - Molecular mechanics calculations (Macromodel in Maestro).
  - Molecular dynamics simulations (LAMMPS, Impact in Maestro).
  - Quantum chemical calculations (Gaussian package, QChem).
- ◆ **Basic programming proficiency:**  
Lua, Mathcad, C/C++.

◆ **Instrument operation and experimentation:**

- Mass spectrometry:
  - Guided ion beam tandem (magnetic sector and quadrupole mass filter) mass spectrometer (home-built).
  - Fourier transform ion cyclotron resonance mass spectrometer (home-built).
  - Quadrupole ion trap mass spectrometer (Finnigan ITMS).
- Ionization sources:
  - Direct current discharge.
  - Electrospray ionization.
- Tandem mass spectrometry:
  - Exchange reactions.
  - Collisional activation (collision-induced dissociation).
  - Blackbody infrared radiative dissociation.
  - Infrared and ultraviolet photo-dissociation.
  - Electron capture dissociation.
- Vacuum systems.
- Super-conducting magnets:
  - Cryogen handling.
- Lasers:
  - Tunable optical parametric oscillator/amplifier system with Nd:YAG pump laser.
  - Excimer laser.
  - CO<sub>2</sub> laser.
- Separation methods:
  - High pressure liquid chromatography.
  - Gas chromatography.

◆ **Languages:**

Fluent in Swedish and Bulgarian, and intermediate in German.

**PUBLICATIONS:**

- 16) Demireva, M.;** Armentrout, P. B. *J. Phys. Chem. A* **2018**, *122*, 750-761.  
“Activation of H<sub>2</sub> by Gadolinium Cation (Gd<sup>+</sup>): Bond Energy of GdH<sup>+</sup> and Mechanistic Insights from Guided Ion Beam and Theoretical Studies”
- 15) Demireva, M.;** Armentrout, P. B. *Top. Catal.* **2017**, <https://doi.org/10.1007/s11244-017-0858-1>.  
“Activation of CO<sub>2</sub> by Gadolinium Cation (Gd<sup>+</sup>): Energetics and Mechanism from Experiment and Theory”
- 14) Armentrout, P. B.;** **Demireva, M.;** Peterson, K. A. *J. Chem. Phys.* **2017**, *147*, 214307(1)-(10).  
“Guided Ion Beam and Theoretical Studies of the Bond Energy of SmS<sup>+</sup>”
- 13) Demireva, M.;** Armentrout, P. B. *J. Chem. Phys.* **2017**, *146*, 174302(1)-174302(13).  
“Gadolinium Cation (Gd<sup>+</sup>) Reaction with O<sub>2</sub>: Potential Energy Surface Mapped Experimentally and with Theory”
- 12) Demireva, M.;** Kim, J.; Armentrout, P. B. *J. Phys. Chem. A* **2016**, *120*, 8550-8563.  
“Gadolinium (Gd) Oxide, Carbide, and Carbonyl Cation Bond Energies and Evaluation of the Gd + O → GdO<sup>+</sup> + e<sup>-</sup> Chemi-Ionization Reaction Enthalpy”

- 11) **Demireva, M.**; Oomens, J.; Berden, G.; Williams, E. R. *ChemPlusChem* **2013**, *78*, 995-1004.  
“The Ionic Hydrogen/Deuterium Bonds between Diammoniumalkane Dications and Halide Anions”
- 10) Gillis, E. A. L.; **Demireva, M.**; Sarwar, M. G.; Chudzinski, M. G.; Taylor, M. S.; Williams, E. R.; Fridgen, T. D. *Phys. Chem. Chem. Phys.* **2013**, *15*, 7638-7647.  
“Structure and Energetics of Gas Phase Halogen-Bonding in Mono-, Bi-, and Tri-dentate Anion Receptors as Studied by BIRD”
- 9) **Demireva, M.**; O’Brien, J. T.; Williams, E. R. *J. Am. Chem. Soc.* **2012**, *134*, 11216-11224.  
“Water-Induced Folding of 1,7-Diammoniumheptane”
- 8) Gillis, E. A. L.; **Demireva, M.**; Nanda, K.; Beran, G.; Williams, E. R.; Fridgen, T. D. *Phys. Chem. Chem. Phys.* **2012**, *14*, 3304-3315. (Cover Article)  
“Structures and Energetics of Electro sprayed Uracil<sub>n</sub>Ca<sup>2+</sup> Clusters ( $n=14-4$ ) in the Gas Phase”
- 7) Donald, W. A.; Leib, R. D.; **Demireva, M.**; Williams, E. R. *J. Am. Chem. Soc.* **2011**, *133*, 18940-18949.  
“Ions in Size-Selected Aqueous Nanodrops: Sequential Water Molecule Binding Energies and Effects of Water on Ion Fluorescence”
- 6) Donald, W. A.; Leib, R. D.; **Demireva, M.**; Negru, B.; Neumark, D. M.; Williams, E. R. *J. Phys. Chem. A*, **2010**, *115*, 2-12.  
“Average Sequential Water Molecule Binding Enthalpies of M(H<sub>2</sub>O)<sup>2+</sup><sub>19-124</sub> (M= Co, Fe, Mn, and Cu) Measured with Ultraviolet Photodissociation at 193 and 248 nm”
- 5) Donald, W. A.; Leib, R. D.; **Demireva, M.**; Negru, B.; Neumark, D. M.; Williams, E. R. *J. Am. Chem. Soc.* **2010**, *132*, 6904-6905.  
“‘Weighing’ Photon Energies with Mass Spectrometry: Effects of Water on Ion Fluorescence”
- 4) **Demireva, M.**; Williams, E. R. *J. Am. Soc. Mass Spectrom.* **2010**, *21*, 1133-1143.  
“Measuring Internal Energy Deposition in Collisional Activation Using Hydrated Ion Nanocalorimetry to Obtain Peptide Dissociation Energies and Entropies”
- 3) Donald, W. A.; **Demireva, M.**; Leib, R. D.; Aiken, M. J.; Williams, E. R. *J. Am. Chem. Soc.* **2010**, *132*, 4633-4640.  
“Electron Hydration and Ion-Electron Pairs in Water Clusters Containing Trivalent Metal Ions”
- 2) Donald, W. A.; Leib, R. D.; **Demireva, M.**; O’Brien, J. T.; Prell, J. S.; Williams, E. R. *J. Am. Chem. Soc.* **2009**, *131*, 13328-13337.  
“Directly Relating Reduction Energies of Gaseous Eu(H<sub>2</sub>O)<sub>n</sub><sup>3+</sup>,  $n = 55-140$ , to Aqueous Solutions: The Absolute SHE Potential and Real Proton Solvation Energy”
- 1) Prell, J. S.; **Demireva, M.**; Oomens, J.; Williams, E. R. *J. Am. Chem. Soc.* **2009**, *131*, 1232-1242.  
“Role of Sequence in Salt-Bridge Formation for Alkali Metal Cationized GlyArg and ArgGly Investigated with IRMPD Spectroscopy and Theory”

## ORAL PRESENTATIONS (given by me):

- 5) **Demireva, M.**; Armentrout, P. B. Lake Arrowhead Ion Chemistry and Mass Spectrometry Conference, Lake Arrowhead, CA, January 15-17, 2016.  
“The  $\text{GdO}^+$  and  $\text{GdO}_2^+$  Bond Energies: Using GIBMS to Map the Potential Energy Surface of the  $\text{Gd}^+$  and  $\text{O}_2$  Reaction”
- 4) **Demireva, M.**; Williams, E. R. 61<sup>st</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Minneapolis, MN, June 9-13, 2013.  
“Effects of Solvation on the Electronic Properties of  $\text{Ru}^{3+/2+/+}(\text{bpy})_3$ ”
- 3) **Demireva, M.**; Williams, E. R. Lake Arrowhead Ion Chemistry and Mass Spectrometry Conference, Lake Arrowhead, CA, January 18-20, 2013.  
“Measuring Relative and Absolute One-Electron Reduction Potentials of Divalent Transition Metal Ions”
- 2) **Demireva, M.**; O’Brien, J. T.; Williams, E. R. 60<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Vancouver, British Columbia, May 20-24, 2012.  
“Water-Induced Folding of Diprotonated 1,7-Diaminoheptane Investigated by IRPD Spectroscopy”
- 1) **Demireva, M.**; Williams, E. R. Lake Arrowhead Ion Chemistry and Mass Spectrometry Conference, Lake Arrowhead, CA, January 14-16, 2011.  
“Internal Energy Distributions of Hydrated Ion Clusters: The Role of Dissociation, Radiative Absorption and Emission”

## POSTER PRESENTATIONS (given by me):

- 7) **Demireva, M.**; Armentrout, P. B. 65<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 4-8, 2017.  
“Energetics and Mechanism of  $\text{CO}_2$  Activation by Gadolinium Cation ( $\text{Gd}^+$ )”
- 6) **Demireva, M.**; Armentrout, P. B. 64<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, San Antonio, TX, June 5-9, 2016.  
“Potential Energy Surface of the  $\text{Gd}^+$  Reaction with  $\text{O}_2$  Mapped with GIBMS and Theory”
- 5) **Demireva, M.**; Kim, J.; Kafle, A.; Armentrout, P. B. 63<sup>rd</sup> ASMS Conference on Mass Spectrometry and Allied Topics, St. Louis, MO, May 31-June 4, 2015.  
“Investigating  $\text{Gd}^+$  Oxidation Reactions and Determining the  $\text{GdO}^+$  Bond Energy Using Guided Ion Beam Mass Spectrometry”
- 4) **Demireva, M.**; Williams, E. R. Gordon Research Conference on Gaseous Ions: Structures, Energetics, and Reactions, Galveston, TX, February 24-March 1, 2013.  
“Reduction vs. Ion-Electron Pairs in Water Clusters Containing Divalent Transition Metal Ions”
- 3) **Demireva, M.**; Williams, E. R. 58<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Salt Lake City, UT, May 23-27, 2010.  
“Dissociation Kinetics of Activated Hydrated Metal Ion Clusters Investigated with Master Equation Modeling”

- 2) **Demireva, M.**; Williams, E. R. Lake Arrowhead Ion Chemistry and Mass Spectrometry Conference, Lake Arrowhead, CA, January 15-17, 2010.  
“Application of Master Equation Modeling to Hydrated Ion Clusters”
- 1) **Demireva, M. P.**; Remes, P. M.; Glish, G. L. 55<sup>th</sup> ASMS Conference on Mass Spectrometry and Allied Topics, Indianapolis, IN, June 3-7, 2007.  
“Internal Energy Relaxation of Different Mass Peptide Ions”

**REFERENCES:**

Available upon request.