

# Ryan Gotchy Mullen

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## EDUCATION

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- University of California, Santa Barbara** 2014  
Ph.D. Chemical Engineering  
Thesis: Mechanisms of rare events in condensed phases
- Brigham Young University** 2006  
B.S. Chemical Engineering, *summa cum laude*

## RESEARCH AND PROFESSIONAL EXPERIENCE

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- Post-doctoral** ■ Lawrence Livermore National Laboratory 2017-present  
Principal investigator: Nir Goldman  
Research interests: actinide surface chemistry, polymer aging, solid-liquid phase equilibrium
- Post-doctoral** ■ University of Notre Dame 2015-2017  
Principal investigators: Edward Maginn, Steven Corcelli  
Research interests: reaction equilibria, ionic liquids
- Graduate** ■ University of California, Santa Barbara 2009-2014  
Advisors: Baron Peters, Joan-Emma Shea  
Research interests: reaction mechanisms, rare events simulation methods, rate theories
- Reservoir Engineer** ■ ExxonMobil, Houston TX  
Interim supervisor, East Texas Reservoir group Jun-Sep 2009  
Reservoir engineer, tight natural gas drillwells and workovers 2006-2009  
Intern 2005

## PUBLICATIONS

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- **RG Mullen**, N Goldman, "Quantum accurate prediction of plutonium-plutonium dihydride phase equilibrium using a lattice gas model" (submitted)
- **RG Mullen**, N Goldman, "A first-principles study of hydrogen surface coverage on  $\delta$ -Pu (100), (111), and (110) surfaces" (in prep)
12. **RG Mullen**, SA Corcelli, EJ Maginn, "Reaction ensemble Monte Carlo simulations of CO<sub>2</sub> absorption in the reactive ionic liquid triethyl(octyl)phosphonium 2-cyanopyrrolide" *Journal of Physical Chemistry Letters* 9.18 5213-5218 (2018)  
<http://dx.doi.org/10.1021/acs.jpcclett.8b02304>
11. QR Sheridan, **RG Mullen**, T Lee, WF Schneider, EJ Maginn, "Predicting CO<sub>2</sub> Solubilities in Aprotic Heterocyclic Anion Ionic Liquids" *Journal of Physical Chemistry C* (2018)  
<http://dx.doi.org/10.1021/acs.jpcc.8b02095>
10. L Lupi, A Hudait, B Peters, M Grunwald, **RG Mullen**, A Nguyen, V Molinero, "Role of Stacking Disorder in Ice Nucleation" *Nature* 551.7679 218-222 (2017)  
<http://dx.doi.org/10.1038/nature24279>

9. BS Yoo, E Marin-Rimoldi, **RG Mullen**, A Jusufi, EJ Maginn, "A Discrete Fractional Component Monte Carlo Simulation Study of Dilute Nonionic Surfactants at the Air-Water Interface" *Langmuir* 33.38 9793-9802 (2017) <http://dx.doi.org/10.1021/acs.langmuir.7b02058>
8. **RG Mullen**, EJ Maginn, "Reaction ensemble Monte Carlo simulation of xylene isomerization in bulk phases and under confinement" *Journal of Chemical Theory and Computation* 13.9 4054-4062 (2017) <http://dx.doi.org/10.1021/acs.jctc.7b00498>
7. JK Shah, E Marin-Rimoldi, **RG Mullen**, ..., EJ Maginn, "Cassandra: An open source Monte Carlo package for molecular simulation." *Journal of Computational Chemistry* 38.19 1727-1739 (2017) <http://dx.doi.org/10.1002/jcc.24807>
6. ZA Levine, MV Rapp, W Wei, **RG Mullen**, C Wu, GH Zerze, J Mittal, JH Waite, JN Israelachvili and J-E Shea, "Surface force measurements and simulations of mussel-derived peptide adhesives on wet organic surfaces" *Proceedings of the National Academy of Sciences* 113.16 4332-4337 (2016) <http://dx.doi.org/10.1073/pnas.1603065113>
5. GH Zerze\*, **RG Mullen\***, ZA Levine\*, J-E Shea and J Mittal, "To what extent does surface hydrophobicity dictate peptide folding and stability near surfaces?" *Langmuir* 31.44 12223-12230 (2015) <http://dx.doi.org/10.1021/acs.langmuir.5b03814>
4. **RG Mullen**, J-E Shea and B Peters, "Easy transition path sampling methods: flexible-length aimless shooting and permutation shooting" *Journal of Chemical Theory and Computation* 11.6 2421-2428 (2015) <http://dx.doi.org/10.1021/acs.jctc.5b00032>
3. **RG Mullen**, J-E Shea and B Peters, "Transmission coefficients, committors, and solvent coordinates in ion-pair dissociation" *Journal of Chemical Theory and Computation* 10.2 659-667 (2014) <http://dx.doi.org/10.1021/ct4009798>
2. **RG Mullen**, J-E Shea and B Peters, "Communication: An existence test for dividing surfaces without recrossing" *Journal of Chemical Physics* 140.4 041104 (2014) <http://dx.doi.org/10.1063/1.4862504>
1. B Peters, PG Bolhuis, **RG Mullen** and J-E Shea "Reaction coordinates, one-dimensional Smoluchowski equations, and a test for dynamical self-consistency" *Journal of Chemical Physics* 138.5 054106 (2013) <http://dx.doi.org/10.1063/1.4775807>

\* contributed equally to this work

## PRESENTATIONS

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| 17. | <b>Berkeley Statistical Mechanics Meeting</b> ■ Berkeley, CA<br>Poster: "Quantum Accurate Prediction of Plutonium-Plutonium Dihydride Phase Equilibrium Using a Spin-Lattice Model" | 2020 |
| 16. | <b>Berkeley Statistical Mechanics Meeting</b> ■ Berkeley, CA<br>Poster: "Spin-lattice model of plutonium hydride nucleation"  | 2019 |

15. **AIChE Annual Meeting** ■ Pittsburgh, PA 2018  
Talk: "Reaction ensemble Monte Carlo simulations of protic ionic liquid formation"  
Poster: "First-principles study of hydrogen dissociation on plutonium hydride"
14. **Foundations of Molecular Modeling and Simulation** ■ Delavan, WI 2018  
Poster: "Reaction ensemble Monte Carlo simulations of xylene isomerization in the bulk and under confinement"
13. **AIChE Annual Meeting** ■ Minneapolis, MN 2017  
Talk 1: "Reaction ensemble Monte Carlo simulations of xylene isomerization in the bulk and under confinement"  
Talk 2: "Reaction Ensemble Monte Carlo: Applications to Ionic Liquids"
12. **Midwest Thermo and Stat Mech** ■ Univ of Notre Dame, South Bend, IN 2017  
Talk: "Reaction ensemble Monte Carlo simulations of xylene isomerization in the bulk and under confinement"
11. **AIChE Annual Meeting** ■ San Francisco, CA 2016  
Talk: "Molecular simulation of CO<sub>2</sub> absorption in the ionic liquid [P<sub>2228+</sub>][2CNpyr-] using reaction ensemble Monte Carlo"
10. **26<sup>th</sup> EUCHEM Conference on Molten Salts and Ionic Liquids** ■ Vienna, Austria 2016  
Talk: "Molecular simulation of CO<sub>2</sub> absorption in the ionic liquid [P<sub>2228+</sub>][2CNpyr-] using reaction ensemble Monte Carlo"
9. **Midwest Thermo and Stat Mech** ■ Miami University, Oxford, OH 2016  
Talk: "Molecular simulation of CO<sub>2</sub> absorption in the ionic liquid [P<sub>2228+</sub>][2CNpyr-] using reaction ensemble Monte Carlo"
8. **AIChE Annual Meeting** ■ Salt Lake City, UT 2015  
Talk 1: "Molecular simulation of CO<sub>2</sub> absorption in the ionic liquid [P<sub>2228+</sub>][2CNpyr-] using reaction ensemble Monte Carlo"  
Talk 2: "Easy transition path sampling in the microcanonical ensemble"
7. **AIChE Annual Meeting** ■ Atlanta, GA 2014  
Talk: "Effect of surface hydrophobicity on the conformational stability of GB1 hairpin"
6. **Chemical Sciences Student Seminar** ■ Santa Barbara, CA 2014  
Talk: "Effect of hydrophobicity on the stability of protein structures"  
→ Travel Grant Award for best presentation, voting by the audience
5. **Amgen-Clorox Annual Graduate Student Symposium** ■ Santa Barbara, CA 2014  
Talk: "Ion pair dissociation: solvent coordinates and reaction rate theories"  
→ Best Talk (Presentation Skills), scoring by industry guests
4. **American Conference on Theoretical Chemistry** ■ Telluride, CO 2014  
Poster: "An existence test for dividing surfaces without recrossing"
3. **AIChE Annual Meeting** ■ San Francisco, CA 2013  
Talk: "A simple test for the existence of dividing surfaces without recrossing"

2. **Mini-Stat Mech Meeting** ■ Berkeley, CA 2013  
Poster: "Grote-Hynes, Pollak and dynamics of the committor in ion pair dissociation"
1. **AIChE Annual Meeting** ■ Minneapolis, MN 2011  
Talk: "Solvent dynamics in ion pair dissociation"

## **HONORS**

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- Best Presentation ■ UCSB Chemical Sciences Student Seminar 2014
- Best Talk (Presentation Skills) ■ UCSB Graduate Student Symposium 2014
- Teaching Assistant of the Year ■ UCSB ChE 2012
- NSF Graduate Research Fellow 2011
- Distinguished Service Award, for dept. recruiting ■ UCSB ChE 2011

## **OUTREACH**

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- Science Olympiad coach ■ Christensen Middle School 2018-present
- Fun With Science presentations to 5<sup>th</sup> graders ■ LLNL 2017-present
- Molecular simulation intro for high school students ■ ND Summer Scholars 2015-2017
- Family science night volunteer ■ Family Ultimate Science Exploration, UCSB 2009-2014
- Math & science tutor for high school students ■ Santa Barbara, CA 2011-2012