

SUSAN REMPE, Ph.D.

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RESEARCH INTERESTS

Biomolecular structure-dynamics-function relationships, membranes for selective transport, ion channels, enzyme-ligand binding & catalysis, solvation & transport theory, ab initio simulations.

PROFESSIONAL PREPARATION

B.A. Premedical Sciences (History and German Concentrations), Columbia University, NY

B.A. Chemistry, University of Montana, MT, *Research Advisor:* Dr. Richard J. Field

M.S. and Ph.D. Chemistry, University of Washington, WA, *Thesis Advisor:* Dr. Robert O. Watts

POSITIONS

Research Professor, Dept. Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico (2015 – present)

Adjunct Professor, Dept. of Biology, University of New Mexico (2014 – present)

Wilmshire Fellow, School of Chemistry, University of Melbourne, Australia (2012)

Distinguished Member of Technical Staff, Sandia National Labs (2012 – present)

Principal, Senior Member of Technical Staff, Sandia National Labs (2006-2011), (2001-2006)

Postdoctoral Fellow, Theoretical Division, Los Alamos National Laboratory (1999-2001)

Visiting Research Scholar, University of Melbourne, Australia (1996)

Graduate Research Associate and Teaching Assistant, University of Washington (1990-1998)

Undergraduate Teaching Assistant, University of Montana (1988-1990)

HONORS & AWARDS

Innovation awards, UNM ('16) and Sandia ('17)

International R&D 100 Gold Award Winner in Green Tech, "CO₂ Memzyme™," *R&D Magazine* ('15)

International R&D 100 Award Winner in Materials, "CO₂ Memzyme™," *R&D Magazine* ('15)

Time Magazine online "The 5 Best Ideas of Today" by the Aspen Institute (05/13, '15)

New Mexico Women of Influence & Overall Government Category Winner, *Alb. Business First* ('15)

Notable Tech. Development Award, Federal Labs Consortium ('12, '14)

Outstanding Women at Sandia ('12, '14)

Intellectual Property Achievement Award, Sandia ('12)

International R&D 100 Award for "Biomimetic Water Purification Membranes," *R&D Magazine* ('11)

Research highlighted by DoE Secretary Chu in "Water Matters" talk, Vienna ('11)

Employee Recognition Award for Individual Technical Excellence, Sandia ('11)

Up and Coming Innovator Award, Sandia ('11)

Outstanding Woman in Technology, New Mexico Technology Council ('11)

Award for Excellence, Laboratory Directed Research & Development, Sandia ('10)

Invited Speaker representing Science & Technology, Fall Leadership Forum Sandia Executives ('07)

Sandia President's Volunteer Service Award for Coaching & Officiating, Kirtland Aquatic Club ('07)

Elected Fellow of the American Academy of Nanomedicine ('06)

Young Investigator Award, American Academy of Nanomedicine ('06)

Profiled in *New Mexico Woman Magazine* as Outstanding Sandia Scientist ('04)

Women's Wall of Fame, Sandia ('04)

DOE Educational Science Prize, UW ('95)

Assoc. for Women in Science & Shell Graduate Research Fellowships, UW ('95)

Ringold Outstanding Graduate Student Fellowship, UW ('90-'96)

American Chemical Society & American Institute of Chemists Undergrad. Dept. Awards, UM ('89)

SYNERGISTIC ACTIVITIES*Organizer:*

- Vice Chair & Chair-Elect, Gordon Research Conference on Water & Aqueous Solutions ('18 - '22)
- Chair, Vice Chair, Secretary/Treasurer Permeation and Transport Subgroup of the BPS ('14 - '19)
- Member-at-Large, Four Corners Meeting of the APS (2015 - 2018)
- Co-Chair, Telluride Science Research Center Workshop on "Ions in Solution: Energy, Biology, and Environment" ('10, '12, '14, '16, '18)
- Chair ACS Symposium on "Hydrophobicity, Ions, & Interfaces," Boston (2015)
- Co-Chair, APS Invited Symposium on "QM Applied to Biophysics Problems," Denver (2014)
- Chair, IEEE Nanotech. Materials & Devices Conference Session, Aci Castello, Italy ('14)
- Discussion Leader, SNL Truman Lecturer (Andre Nel, UCLA) (2012)
- Organizer & Chair, Sandia's Bioscience & Tech. Conference (2009)
- Organizer and Host, Sandia's BioMaterials Science Symposium, 29 visitors (2007-current)
- Co-Organizer and Co-Chair, International Symposium on "Ions in Complex Environments," American Chemical Society Meeting in Washington, DC (2005)
- Chair, Symp. on "Classical and Statistical Studies of Solvation," Pacifichem, Hawaii ('05)

Reviewer:

- *PNAS, J Gen Physiol, JACS, PRL, Biophys J, J Chem Phys, Biophys Chem, Biophys Biochim Acta, J Phys Chem, Phys Chem Chem Phys, J Molec Model, Chem Phys Lett, Sci Rep*
- SNL Proposals (LDRD), R&D 100 Nominations, Truman Fellows (2005-current)
- Proposals to *Petroleum Research Fund* (ACS), DOE SBIR & BES, *Biotech & Bio Sciences RC* (UK)
- DOE/BES Program at Pacific Northwest National Lab (2013)
- Proposals to Netherlands Foundation for Fundamental Research on Matter (2011)
- Member, Inaugural NSF Study Section on Chemistry of Life Processes (2009)
- *Ad hoc* reviewer, NIH Challenge Grants (2009) and NSF (2010-current)

Intellectual Property:

- U.S. patent (2016, 9,242,210) "Enzymatically active high selectivity gas-permeable membranes"
- U.S. patent (2016, 9,486,742) "Biomimetic membranes and methods of making them"

Teaching:

- Developer and Teaching Assistant, UW's First Computational Chemistry Course with Profs. H. Jonsson, R. Heller, W. Reinhardt (1993-1996; won DOE Prize for Science Education)
- Computational exercise on molecular vibrations published in *The Chemical Educator* (1998)
- Teaching Assistant for General, Organic, and Physical Chemistry labs and lectures ('89-'98)

Professional Memberships & Service:

- Member, Board of Directors, Governance Committee, Telluride Science Research Center ('18 - present)
- Discussion Leader, "Biomimetic design," Gordon Research Conference on Water & Aqueous Solutions, NH ('18)
- Discussion Leader, "Protein dynamics from single-particle cryo-EM and from AFM," Telluride Conference on Protein Dynamics, Les Houches, France ('18)
- Discussion Leader and Career Panelist, "Biomolecular systems," Gordon Research Conference & Gordon Research School on Chemistry & Physics of Liquids, Holderness, NH ('17) (decl)
- Chair, Permeation & Transport Subgroup of Biophys. Soc. ('18 - present)
- Vice Chair, Permeation & Transport Subgroup of Biophys. Soc. ('16 - '18)
- Member-at-Large, Executive Committee, 4 Corners Section, APS (2015-present)
- Secretary & Treasurer, Permeation & Transport Subgroup, Biophys. Soc. ('14 - '16)
- Appointed Member, Officer Nominating Committee, Division of Computation, APS ('14 - '16)
- Member Biophys. Soc., Am. Chem. Soc., Electrochem. Soc., Am. Ind. & Chem. Eng. Soc., Am. Acad. Nanomed., Am. Phys. Soc., AAAS, Am. Soc. Biochem. Molec. Biol.

Citizenship & Committee Membership:

- Member, Thesis Committee for Civil Eng. graduate student, UT El Paso ('18 - present)
- Member, Thesis Committee for Chemical Eng. graduate student, Tulane ('16 - present)
- Chair, BioScience Educational Symposium Committee, Sandia ('16 - present)
- Energy & Water Nexus Committee, formed by Geoscience Director, Peter Davies ('16 - present)
- Committee on Academic Ethics, formed by Vice President for Research, UNM ('15, decl.)
- Red Team to evaluate Center for Integrated Nanotechnology DOE/BES proposal ('15)
- SNL Bioscience Center Committees: Diversity, Postdocs, NanoBio Strategy, Science Strategy, BioMaterials Focus Group, Basic Bio Research Strategy ('07-present)
- SNL Materials Sci. Bio Strategy, Detection at Limit & Bio Research Challenges ('14)
- Interview Committees: Bio & Mater'ls Science Center Director (8600), Senior Manager (8630), Biotech. & Bioeng. Dept. Manager (8621), Bioenergy Staff (8621)
- Steering Committee, NIH Nanomedicine Center ('06 – '09)
- Sandia Internal (LDRD) Proposal Reform Committee ('04)
- Research Library Advisory Board, Los Alamos National Laboratory ('99 – '01)

Journal Editor:

- Guest Editor, Special issue on "Ions" with B. Roux for *Biophysical Chemistry* ('06)

Extracurriculars:

- Amateur Concert Pianist, performed at UNM Keller Hall (2003 Spring & Fall, 2006, 2009)
- Volunteer Swim Coach and Official (2004 – 2012)
- Volunteer for Columbia U. as Fundraiser & Summer Internship point of contact (2000 – 2016)

SELECTED INVITED RESEARCH TALKS: Over 100 invited research presentations.

2018 Chemical engineering, U. Pitt.	2014 ACS symposium honoring Rasaiah, CA
2018 Chemical engineering, Columbia U.	2014 Gordon Research Conf. on membranes, NH
2018 Interfacial structure & dynamics, Telluride	2014 Purdue U Chemistry seminar, Indiana
2018 CECAM Ions in the brain, IT	2014 APS symposium on QM for bio, Denver
2018 Protein dynamics Telluride Conf., Les Houches	2014 Singapore Water Conf., Singapore (decl)
2018 Ions in solution, Telluride	2013 Ion channel biophysics workshop, Telluride
2018 GRC molecular & ionic clusters, IT	2013 Aspen biophysics workshop, Aspen
2017 WattsFest2017 honoring R. O. Watts, Sydney	2013 UPS science seminar, Tacoma, WA
2017 University of Pittsburgh, PA (decl)	2012 Tulane Chemistry seminar, New Orleans
2017 Ion channel biophysics, Telluride (decl)	2012 Faraday Disc on ions (poster, declined), UK
2017 U Paris Descartes, France	2012 Ions & molec biology, Telluride
2017 Institut Lumiere Matiere, U Lyon, France	2012 Gordon Research Conf. on water, NH
2017 UNM Health sciences, Abq (decl)	2012 ACS liquid interfaces symposium, Phil.
2016 LBNL Lawrence Seminar, Berkeley	2012 CECAM Conf on Free Energy (Pratt), Paris
2016 Int'l Conf Molec Sim (contrib.), Shanghai, China	2012 Melbourne U Chemical Soc seminar, Melbourne
2016 SNL Bioscience External Review, CA	2012 UW Multidisciplinary seminar, Seattle
2016 Telluride workshops (2), Telluride	2012 Mardi Gras Conf keynote speaker, Baton Rouge
2016 Weill (Cornell) Med. College, New York	2011 Stud. Conf on Water in Bio (Pratt), France
2016 ASU Center for Biophysics, AZ	2011 MRS Nanomaterials symp (Brinker), Boston
2015 Pacificchem interfaces, solvation (2), HI	2011 U of S Florida physics colloquium, Tampa
2015 Sandia Women's Action Network, Abq	2011 UNM Health Sciences Center, Albuquerque
2015 ACS nat. meeting, polymers, ions (2), Bost.	2011 Ion channel biophysics workshop, Telluride
2015 Ion channel biophysics workshop, Telluride	2011 Institute for Pure & App Math, UCLA
2015 UNM Cancer Retreat, Abq	2011 Materials Science Cent. external rev., SNL
2015 SNL Bioscience External Review, Abq	2010 Pacificchem Liquid interfaces symp., HI
2015 ACS Polymer Membranes, Asilomar (decl)	2010 Workshop on ions & molec. bio., Telluride
2015 UNM CETI immunology group, Alb.	2010 EFRC workshop, Santa Fe, NM
2014 Vogel group, ETH, Zurich	2010 American Water Works Assoc., Albuquerque
2014 IEEE Nanotech mat & devices, Sicily	2010 NIH Nanomedicine Centers review, CA
2014 Ions workshop, Telluride	2009 Hope College, WI; Calvin College, WI

2009 Ion channel biophysics workshop, Telluride
 2009 ACS Polarizable force fields symp., SLC
 2009 BPS Permeation & transport group, Boston
 2009 Weill (Cornell) Med. College, New York City
 2009 Bioscience and Tech. Forum, Albuquerque
 2008 MERCURY Keynote speaker, Hamilton Coll.
 2008 U Maryland Biology Dept., College Park, MD
 2008 International School for Adv. Studies, Italy
 2008 Wolfgang Pauli Institute, Vienna
 2008 U Minnesota Chemistry Dept., Minneapolis
 2008 AAAS Southwest regional meeting, Alb.
 2007 Brandeis U. Chemistry Dept., MA
 2007 Nano-bio workshop on membranes, UI-UC
 2007 NIH Nanomedicine Cent. review, Indianap.
 2007 NIH Nanomedicine Cent. review, Bethesda
 2007 BPS ion channels workshop, Baltimore, MD
 2007 Rush U. Medical Center, Chicago, IL
 2007 UNM Health Sciences Center, Alb.
 2007 Bioscience Center external review, Alb.
 2006 Materials Research Society (MRS), Boston
 2006 UI Biology Dept., Urbana-Champaign, IL
 2006 NIH Nanomedicine Center review, UI-UC
 2006 Americ. Acad. of Nanomedicine, Wash., DC
 2006 The Mind Institute, UNM, Albuquerque
 2006 Sandia-Livermore seminar, Livermore
 2005 Pacifichem Interfaces symposium, HI
 2005 Pacifichem Solvation symposium, HI
 2005 AIChE, Cincinnati
 2005 Pacific Northwest National Laboratory
 2004 Beckman Institute, UI-UC
 2004 Electrochemical Society, HI
 2003 U of Houston Chemistry Dept., TX
 2003 Electrochemical Society, Paris
 2001 Carleton College Chemistry Dept., MN
 2001 U Montana Chemistry Dept., Missoula, MT
 2001 Cal State Chemistry Dept., Long Beach
 2001 ICCN Computational nanoscience, NC
 2001 Sandia National Labs, Surface science, Alb.
 2001 ACS Molecular aq. environments, San Diego
 2000 Motorola, Los Alamos
 2000 Pacifichem Ion channels symposium, HI
 2000 NIST Thermophysical properties, Boulder
 2000 ACS Frontiers in biophys. theory, Wash., DC
 1998 Los Alamos National Laboratory
 1998 Sandia National Labs, Comput. Cent., Alb.
 1995 DOE Awards ceremony, Washington, DC

SELECTED RECENTLY FUNDED RESEARCH ACTIVITIES:

External

- **DTRA JSTO-CBD (CB10412)**, "Polymerization and in situ neutralization of chemical warfare agents," co-PI, (10/1/2017 - 9/30/2020).
- **DOE Technology Commercialization Fund**, "Memzyme Technology for Cost-Effective CO₂ Separations in Enhanced Oil Recovery," PI, (4/1/2018 - 3/31/2020).
- **DTRA JSTO-CBD**, "Advanced therapeutics for exotoxins based on multi-functional mechanistic design principles," PI, (6/15/2016 - 9/30/2018).
- **DTRA JSTO-CBD**, "Understanding selective field-biased gating of biopolymers at confining nanopores," co-PI, (9/15/2012 - 9/30/2018).
- **DOE Battery Materials Research Program**, "First principles modeling of SEI formation on bare and surface/additive modified silicon anode," co-PI, (2/2013-2/2017).
- **NSF CHE-1301072**, "The effects of charge transfer on aqueous and ionic systems," co-PI with UNO, (7/1/2013 - 6/30/2017).
- **DOE/BES (DE-FG02-02-ER15368)**, "Catalytic and transport behaviors of model and porous and composite nanostructures," team member, (11/2012 - 11/2014).
- **AFOSR (FA9550-10-1-0054)**, "Biocompatible and biomimetic self-assembly of functional nanostructures," team member, (10/1/2013 - 9/30/2016).
- **DTRA JSTO-CBD**, "Enhancing enzymatic activity," team member, (9/1/2013 - 8/30/2014).
- **California Proposition 50 Program**, "Hybrid electrodeionization for selective removal of arsenic, nitrate, and perchlorate ions," co-PI, (approved, not funded).
- **NIH Nanomedicine Roadmap**, "Design of biomimetic nanoconductors," co-PI (10/01/2005 - 9/30/2011).
- **DTRA JSTO-CBD (#CBS.FATE.03.10.SN.002)**, "Developing a molecular understanding of water-CWA-surface interactions," co-PI, (2/2010-9/2011).
- **Institut Laue-Langevin**, "Ion hydration structure," co-PI, neutron beam time (07 - 09).
- **Petroleum Research Fund**, "ACS symposium on ions in water," co-PI, (8/01/2005-9/01/2005).
- **National Science Foundation** Summer Undergraduate Research Grant, UM (89)

SELECTED PUBLICATIONS

Author of more than 80 peer-reviewed scientific articles available on Google Scholar.

<https://scholar.google.com/citations?user=9d0L-m4AAAAAJ&hl=en>

1. Muralidharan, A; Chaudhari, MI; Pratt, LR and **SB Rempe**. 2018. Quasi-chemical theory with cluster sampling from ab initio molecular dynamics: Fluoride (F⁻) hydration. *J. Phys. Chem. B* (invited for Special Issue in honor of William P. Reinhardt) (submitted)
2. Ma, P; Cardenas, AE; Chaudhari, MI; Elber, R; and **SB Rempe**. 2018. Mutations of the anthrax channel affect translocation: Atomically detailed simulations with milestone. *J. Phys. Chem. B* (submitted).
3. Percival, S; Small, L; Spoerke, E; and **SB Rempe**. 2018. Polyelectrolyte layer-by-layer deposition on nanoporous supports for ion-selective membranes. *RSC Adv.* (in print).
4. Wen, P-C; Vanegas, JM; **Rempe, SB**; and E Tajkhorshid. 2018. Probing key elements of teixobactin-lipid II interactions in membrane. *Chem. Sci.* 9:6997-7008.
5. Fan, C; Jiang, G; Tian, Y; Gao, Y; **Rempe, SL**, and YB Jiang. 2018. Achieving uniform and conformal ALD coatings on sub-10nm pores using dual-stage exposure/ purge at optimized growth temperatures. *MRS Advances*, 351:1-7.
6. Muralidharan, A; Pratt, LR; Hoffman, GG; Chaudhari, MI; and **SB Rempe**. 2018. Molecular simulation results on charged carbon-nanotube forest supercapacitors. *ChemSusChem*. 11 (invited; <https://doi.org/10.1002/cssc.201800323>).
7. Gao, A; Tan, L; Chaudhari, MI; Asthagiri, D; Pratt, LR; **Rempe, SB**; and JD Weeks. 2018. The role of solute attractive forces in the atomic-scale theory of hydrophobic effects. *J. Phys. Chem. B* 122:6272-76.
8. Muralidharan, A; Chaudhari, MI; Pratt, LR. and **Rempe, SB**. 2018. Molecular dynamics of lithium ion transport within a model solid electrolyte interphase. *Sci. Rep.* 8:10736.
9. Vermaas, JV; **Rempe, SB**; and E Tajkhorshid. 2018. Electrostatic lock in the transport cycle of the multi-drug resistance transporter EmrE. *Proc. Nat. Acad. Sci. USA* 115:E7502-11 (accompanied by [Commentary PNAS \(2018\) 115:8061](#)).
10. Chaudhari, MI and **SB Rempe**. 2018. Strontium and barium in aqueous solution and a potassium channel binding site. *J. Chem. Phys.* 148:222831 (invited for Special Topic Issue on Ions in Water).
11. Baker, CA; Schudel, B; Chaudhari, MI; Wu, K; Dunford, DE; **Rempe, SB**; and AV Hatch. 2018. Nanoporous hydrogels for the observation of anthrax exotoxin translocation dynamics. *ACS Appl. Mater. Interfaces* 10:13342-49.
12. Muralidharan, A.; Pratt, L.R; Chaudhari, MI; and **SB Rempe**. 2018. Comparison of single-ion molecular dynamics in common solvents. *J. Chem. Phys.* 148:222821 (invited to Special Topic Issue on Ions in Water).
13. Fu, Y; Jiang, Y-B; Dunphy, D; Xiong, H; Coker, E; Chou, S; Zhang, H; Vanegas, J; Croissant, J; Cecchi, JL; **Rempe, SB** and CJ Brinker. 2018. Ultra-thin enzymatic liquid membrane for CO₂ separation and capture. *Nat. Commun.* 9:990 (accompanied by [News & Views Nature Energy \(2018\)](#)).
14. Vanegas, J; Heinrich, F; Rogers, DM; Carson, B; La Bauve, S; Vernon, BC; Akgun, B; Satja, S; Zheng, A; Kielian, M; **Rempe, SB**; and MS Kent. 2018. Insertion of Dengue E into lipid bilayers by neutron reflectivity and molecular dynamics simulations. *BBA: Biomembranes* 1860:1216-1230.
15. Chaudhari, MI; Muralidharan, A.; Pratt, LR; and **SB Rempe**. 2018. Molecular simulations of non-aqueous electrolyte solutions. *Top. Curr. Chem. (Z)* 376:7 (invited review for Special Issue on Modeling Electrochemical Energy Storage at the Atomic Scale, ed. Martin Korth, Springer).
16. Chaudhari, MI; Pratt, LR; and **SB Rempe**. 2018. Utility of chemical computations in predicting solution free energies of metal ions. *Mol. Simul.* 44:110-116 (invited Special Issue "Proceedings of the 4th International Conference on Molecular Simulation").
17. Ma, P; Cardenas, A; Chaudhari, MI; Elber, R; and **SB Rempe**. 2017. The impact of protonation on early translocation of anthrax lethal factor: Kinetics from molecular dynamics simulations and milestone theory. *J. Am. Chem. Soc.* 139:14837-14840.
18. Chaudhari, MI; **Rempe, SB**; and LR Pratt. 2017. Quasi-chemical theory of F⁻(aq): The 'no split occupancies rule' revisited. *J. Chem. Phys.* 147:161728 (invited; Special Topic on From Quantum Mechanics to Force Fields with Guest Editors Ken Jordan and Jean-Philip Piquemal).
19. VanGordon, MR; Gyawali, G; Rick, SW; and **SB Rempe**. 2017. Atomistic study of intramolecular interactions in the closed-state channelrhodopsin chimera, C1C2. *Biophys. J.* 112:945-952.
20. Stevens, MJ; and **SLB Rempe**. 2016. Ion-specific effects in carboxylate binding sites. *J. Phys. Chem. B* 120:12519-12530.

21. Chaudhari, MI; Pratt, LR; Soto, F; Balbuena, P; and **SB Rempe**. 2016. Scaling atomic partial charges of carbonate solvents for lithium ion (Li^+) solvation and diffusion. *J. Chem. Theory Comput.* 12:5709-5718.
22. La Bauve, E; Vernon, BC; Ye, D; Rogers, D; Siegrist, CM; Carson, B; **Rempe, SL**; Zheng, A; Kielian, M; Shreve, AP; and MS Kent. 2016. Method for measuring the unbinding energy of strongly-bound membrane-associated proteins. *BBA: Biomembranes* 1858:2753-2762.
23. Pratt, LR; Chaudhari, MI; and **SB Rempe**. 2016. Statistical analyses of hydrophobic interactions: A mini-review. *J. Phys. Chem. B (Mini-Review)* 120:6455-6460 (invited; cover, [ACS Editor's choice](#), [video](#)).
24. You, X; Chaudhari, MI; **Rempe, SB**; and LR Pratt. 2016. Dielectric relaxation of ethylene carbonate and propylene carbonate from molecular dynamics simulations. *J. Phys. Chem. B* 120:1849-53 (invited Bruce Garrett Festschrift).
25. Chaudhari, MI; **Rempe, SB**; Asthagiri, D; Tan, L; and LR Pratt. 2016. Molecular theory and the effects of solute attractive forces on hydrophobic interactions. *J. Phys. Chem. B* 120:1864-70 (invited Bruce Garrett Festschrift).
26. You, X; Chaudhari, MI; **Rempe, SB**; and LR Pratt. 2015. Dielectric properties of ethylene carbonate and propylene carbonate using molecular dynamics simulations. *ECS Trans.* 69:107-111.
27. Anishkin, A; Vanegas, J.; Rogers, DM; Lorenzi, PL; Chan, WK; Purwaha, P; Weinstein, J; Sukharev, S; and **SB Rempe**. 2015. Catalytic role of the substrate defines specificity of therapeutic L-asparaginase. *J. Mol. Bio.* 427:2867-85.
28. Chaudhari, MI; Soniat, M; and **SB Rempe**. 2015. Octa-coordination and the aqueous Ba^{2+} ion. *J. Phys. Chem. B* 119:8746-53.
29. Soniat, M; Rogers, DM; and **SB Rempe**. 2015. Dispersion- and exchange-corrected density functional theory for sodium ion hydration. *J. Chem. Theory Comput.* 11:2958-67.
30. Leung, K; Chaudhari, MI; **Rempe, SB**; Fenton, KR; Pratt, HD; Staiger, CL; and G. Nagasubramanian. 2015. Density functional theory and conductivity studies of boron-based anion receptors. *J. Electrochem. Soc.* 162:A1927-34.
31. Mason, PE; Ansell, S; Neilson, GW; and **SB Rempe**. 2015. Neutron scattering studies of the hydration structure of $\text{Li}^+(\text{aq})$. *J Phys Chem B* 119:2003-9.
32. Rogers, DM; Kent, M; and **SB Rempe**. 2015. Molecular basis of host-membrane association for the Dengue virus envelope protein. *Biochim. Biophys. Acta – Biomembranes* 1848:1041-52.
33. Chaudhari, MI; Sabo, D; LR Pratt; and **SB Rempe**. 2014. Hydration of $\text{Kr}(\text{aq})$ in dilute and concentrated solutions. *J. Phys. Chem. B* 119:9098-9102 (invited Branka Ladanyi Festschrift).
34. Fu, Y; Li, B; Jiang, Y-B; Dunphy, DR; Tsai, A; Tam, S-Y; Li, B; Fan, H; Zhang, H; Rogers, DM; **Rempe, SB**; Atanassov, P; Cecchi, JL; and CJ Brinker. 2014. Atomic layer deposition of L-alanine polypeptide. *J. Am. Chem. Soc.* 136:15821-24.
35. Andersen, M; Rogers, DM; Mai, J; Schudel, B; Hatch, A; **Rempe, SB**; and A Mani. 2014. Spatiotemporal pH dynamics in concentration polarization near ion-selective membranes. *Langmuir* 30:7902-12.
36. Chan, WK; Lorenzi, PL; Anishkin, A; Purwaha, P; Rogers, DM; Sukharev, S; **Rempe, SB**; and JN Weinstein. 2014. The glutaminase activity of L-asparaginase is not required for anticancer activity against ASNS-negative cells. *Blood* 123:3596-3606.
37. Leung, K; **Rempe, SB**; Foster, ME; Ma, Y; Martinez del la Hoz, J; Sai, N and PB Balbuena. 2014. Modeling electrochemical decomposition of fluoroethylene carbonate on silicon anode surfaces in lithium ion batteries. *J. Electrochem. Soc.* 161:A213-21.
38. Rossi, M; Tkatchenko, A; **Rempe, SB**; and S Varma. 2013. The role of methyl-induced polarization in ion binding. *Proc. Natl. Acad. Sci. USA* 110:12978-83.
39. Sabo, D.; Jiao, D.; Varma, S.; Pratt, LR and **SB Rempe**. 2013. Case study of $\text{Rb}^+(\text{aq})$, quasi-chemical theory of ion hydration, and the *no split occupancies* rule. *Ann. Rep. Prog. Chem., Sect C: Phys. Chem.* 109:266 (commissioned by the Royal Society of Chemistry, UK).
40. Jiao, D; and **SB Rempe**. 2012. Combined DFT and continuum calculations of pK_a in carbonic anhydrase. *Biochem.* 51:5979-89.
41. Rogers, DM; and **SB Rempe**. 2012. Reply to "Comment on `Probing the thermodynamics of competitive ion binding using minimum energy structures.'" *J. Phys. Chem. B* 116:7994-995.
42. Rogers, DM; and **SB Rempe**. 2012. Irreversible thermodynamics. *J. Phys.: Conf. Ser.* 401:012014.
43. Varma, S; Rogers, DM; Pratt, LR; and **SB Rempe**. 2011. Design principles for K^+ selectivity in membrane transport. *J. Gen. Physiol. (Perspectives on Ion Selectivity)* 137:479-88 (invited).

44. Alam, TM; Hart, D; and **SLB Rempe**. 2011. Computing the ^7Li NMR chemical shielding of hydrated Li^+ using cluster calculations and time-averaged configurations from ab initio molecular dynamics simulations. *Phys. Chem. Chem. Phys.* 13:13629 ([back cover](#)).
45. Jiao, D; and **SB Rempe**. 2011. CO_2 solvation free energy using quasi-chemical theory. *J. Chem. Phys.* 134:224506-17.
46. Rogers, DM; and **SB Rempe**. 2011. Probing the thermodynamics of competitive ion binding using minimum energy structures. *J. Phys. Chem. B* 115:9116–9129.
47. Rogers, DM; Beck, TL; and **SB Rempe**. 2011. An information theory approach to nonlinear, non-equilibrium thermodynamics. *J. Statistical Phys.* 145:385-409 ([invited](#)).
48. Jiao, D; Leung, K; **Rempe, SB**; and TM Nenoff. 2011. First principles calculations of atomic nickel redox potentials and dimerization free energies: A study of metal nanoparticle growth. *J. Chem. Theory Comput.* 7:485-495.
49. Varma, S; and **SB Rempe**. 2010. Multi-body effects in ion binding and selectivity. *Biophys. J.* 99:3394.
50. Asthagiri, D; Dixit, PD; Merchant, S; Paulaitis, M; Pratt, LR; **Rempe, SB**; and S Varma. 2010. Ion selectivity from local configurations of ligands in solutions and ion channels. *Chem. Phys. Lett. (Frontiers Article)* 485:1-7 ([invited](#), [cover](#), [dedicated feature on journal website](#)).
51. **Rempe, SB**; and K Leung. 2010. Response to “Comment on ‘Ab initio molecular dynamics calculation of ion hydration free energies’ [JCP 133, 047103 (2010)].” *J. Chem. Phys.* 133:047104.
52. Davis, RW; Aaron, JS; **Rempe, SL**; and JA Timlin. 2010. Fluorescence fluctuation analysis of mixed chromophores from a line-scanning hyperspectral imaging system. *Proc. SPIE* 7570 (757002):1-11.
53. Lorenz, CD; Tsige, M; **Rempe, SB**; Chandross, M; Stevens, MJ; Grest, GS. 2010. Simulation study of the silicon oxide and water interface. *J. Comput. Theor. Nanosci.* 7(12):2586-2601 ([invited](#)).
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- Progress toward plugging an antibiotic pump ([LabNews](#), Aug. '18)
- Sandia's nano-stabilized enzymatic membrane for CO₂ capture: [video](#), Lab News ('18)
- Sandia's biomimetic membranes for water purification: [video](#)
- Sandia Recruiting [Video](#)
- Sandia President State of Labs Address ('11, '15)
- *Sandia Research Magazine* ('06, '15, Aug. '16)
- *Sandia Lab News* ('06; '11; '12; '14; March, [May](#), October, [November](#) '15; [Sept.](#) '16)
- *Sandia LDRD Annual Report* ('14); *Sandia Partnerships Annual Report FY2013* ('14)
- *Sandia Lab Accomplishments* ('12, '13, '16, '17)
- *Sandia's High-Performance Computing Annual Reports* (two in '13, three in '14, one in '15, two in '16)
- *Sandia Executive Report to Congress* ('09)
- *Science Matters* ('07)

- *Sandia LDRD Program Review* ('06)

Selected External Publicity

- [News Release](#) on countering bacterial resistance to antimicrobial compounds ('18)
- [News Release](#) on bio-inspired CO₂ capture membranes ('18)
- Albuquerque, the Magazine (Oct. '18)
- *Commentary* ([PNAS, 2018](#))
- Nature News & Views article ([Nature Energy, 2018](#))
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- *Abq J*, *UNM Newsroom*, [energy.sandia.gov](#), DOE's [energy.gov](#) ('15)
- Biophysical Society *New & Notable* article (*Biophys J* (2007) 93:1091-92) ('07)
- *Chemical and Engineering News* 78:42 ('00)