Brian K. Radak

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Research Experience

2017- University of Illinois at Urbana–Champaign Postdoctoral Researcher, Advisor: Emad Tajkhorshid
2017- University of Maryland, Baltimore Visiting Affiliate, Host: Alexander MacKerell

- pH and protonation state effects on protein-lipid interactions
- Software development: alchemical free energy and integrator methodologies

2015-2017 Argonne Leadership Computing Facility Postdoctoral Appointee, Theta Early Science Program
2014-2015 University of Chicago Postdoctoral Scholar, Advisor: Benoît Roux

- Development of constant pH molecular dynamics methods utilizing non-equilibrium MD/MC
- Protonation effects on conformation and binding in P-type ATPases

2011-2014 Rutgers University Visting Scholar/Graduate Assistant
2009-2011 University of Minnesota Graduate Assistant, Advisor: Darrin M. York

- Molecular dynamics simulations of reaction mechanisms, metal binding, and pK_a shifts in ribozymes
- Maximum likelihood methods for constructing free energy profiles from simulations
- Analysis of KIEs of model RNA systems, ribonucleases, and ribozymes
  Collaborators: Michael E. Harris (Case Western Reserve Univ.), Joseph A. Piccirilli (Univ. of Chicago)
- Novel asynchronous replica exchange simulation schemes on distributed cyberinfrastructure
  Collaborators: Ronald M. Levy, Shantenu Jha (Rutgers Univ.)

Education

2008-2014 University of Minnesota, College of Science and Engineering
Doctor of Philosophy, Chemical Physics, Advisor: Darrin M. York
Dissertation: Computational Methods for Understanding RNA Catalysis: A Molecular Approach

2004-2008 Northwestern University, Weinberg College of Arts and Sciences
Master of Science, Chemistry, Advisor: George C. Schatz
Bachelor of Arts, Integrated Science (w/honors) and Chemistry
Honors Thesis: A Theoretical Study of Exothermic Reactive Scattering at the Gas-Liquid Interface: F(^{2}P) + Squalane

Publications

1. **Radak, B. K.**; Suh, D.; Roux, B. A Generalized Linear Response Framework for Expanded Ensemble and Replica Exchange Simulations. *J. Chem. Phys.* **2018**, *149*, 072315.
2. Suh, D.; **Radak, B. K.**; Chipot, C.; Roux, B. Enhanced Configurational Sampling with Hybrid Non-Equilibrium Molecular Dynamics–Monte Carlo Propagator. *J. Chem. Phys.* **2018**, *148*, 014101.

3. **Radak, B. K.**; Chipot, C.; Suh, D.; Jo, S.; Jiang, W.; Phillips, J. C.; Schulten, K.; Roux, B. Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. *J. Chem. Theory Comput.* **2017**, *13*, 5933–5944.

4. Huang, M.; Dissanayake, T.; Kuechler, E.; **Radak, B. K.**; Lee, T.-S.; Giese, T. J.; York, D. M. A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. *J. Chem. Theory Comput.* **2017**, *13*, 3975–3984.

5. **Radak, B. K.**; Roux, B. Efficiency in Nonequilibrium Molecular Dynamics Monte Carlo Simulations. *J. Chem. Phys.* **2016**, *145*, 134109.

6. Lee, T.-S.; **Radak, B. K.**; Harris, M. E.; York, D. M. A Two Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. *ACS Catalysis* **2016**, *6*, 1853–1869.

7. **Radak, B. K.**; Lee, T.-S.; Harris, M. E.; York, D. M. Assessment of Metal-Assisted Nucleophile Activation in the Hepatitis Delta Virus Ribozyme from Molecular Simulation and 3D-RISM. *RNA* **2015**, *21*, 1566–1577.

8. Panteva, M. T.; Dissanayake, T.; Chen, H.; **Radak, B. K.**; Kuechler, E. R.; Giambaşu, G. M.; Lee, T.-S.; York, D. M. Multiscale Methods for Computational RNA Enzymology. *Methods Enzymol.* **2015**, *553*, 335–374.

9. **Radak, B. K.**; Romanus, M.; Lee, T.-S.; Chen, H.; Huang, M.; Treikalis, A.; Balasubramanian, V.; Jha, S.; York, D. M. Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. *J. Chem. Theory Comput.* **2015**, *11*, 373–377.

10. Lee, T.-S.; **Radak, B. K.**; Wong, K.-Y.; York, D. M. Roadmaps Through Free Energy Landscapes Calculated Using the Multi-Dimensional vFEP Approach. *J. Chem. Theory Comput.* **2014**, *10*, 24–34.

11. Giese, T. J.; Chen, H.; Dissanayake, T.; Giambaşu, G. M.; Heldenbrand, H.; Huang, M.; Kuechler, E. R.; Lee, T.-S.; Panteva, M. T.; **Radak, B. K.**; York, D. M. A Variational Linear-Scaling Framework to Build Practical, Efficient Next-Generation Orbital-Based Quantum Force Fields. *J. Chem. Theory Comput.* **2013**, *9*, 1417–1427.

12. **Radak, B. K.**; Romanus, M.; Gallicchio, E.; Lee, T.-S.; Weidner, O.; Deng, N.-J.; He, P.; Dai, W.; York, D. M.; Levy, R. M.; Jha, S. A Framework for Flexible and Scalable Replica-Exchange on Production Distributed Cyberinfrastructure. In *XSEDE '13*, Proceedings of the Conference on Extreme Science and Engineering Discovery Environment: Gateway to Discovery, San Diego, CA, July 22-25; ACM: New York, 2013.

13. Gu, H.; Zhang, S.; Wong, K.-Y.; **Radak, B. K.**; Dissanayake, T.; Kellerman, D. L.; Dai, Q.; Miyagi, M.; Anderson, V. E.; York, D. M.; Piccirilli, J. A.; Harris, M. E. Experimental and Computational Analysis of the Transition State for Ribonuclease A-Catalyzed RNA 2'-*O*-Transphosphorylation. *Proc. Natl. Acad. Sci. USA* **2013**, *110*, 13002–13007.

14. Lee, T.-S.; **Radak, B. K.**; Pabis, A.; York, D. M. A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. *J. Chem. Theory Comput.* **2013**, *9*, 153–164.

15. **Radak, B. K.**; Harris, M. E.; York, D. M. Molecular Simulations of RNA 2'-*O*-Transesterification Reaction Models in Solution. *J. Phys. Chem. B* **2013**, *117*, 94–103.

16. **Radak, B. K.**; Yockel, S.; Kim, D.; Schatz, G. C. Modeling Reactive Scattering of F(^{2}P) at a Liquid Squalane Interface: A Hybrid QM/MM Molecular Dynamics Study. *J. Phys. Chem. A* **2009**, *113*, 7218–7226.

Conference Presentations and Invited Talks

Radak, B. K. Transition Path Sampling Methods and Constant pH Simulations, *NAMD "Hands-On" Workshop: Enhanced Sampling and Free-Energy Calculation*, Urbana, IL, Sept. 25–29, **2017**.

Radak, B. K. Expanded Ensemble Simulations with NAMD: Free Energies, Enhanced Sampling, and Constant pH, *NAMD Developer Workshop*, Chicago, IL, May 22, **2017**. Invited.

Radak, B. K.; Phillips, J. C.; Jiang, W.; Schulten, K.; Roux, B. Constant-pH Simulations on Capability Class Computers: First Applications, *ACS 253rd National Meeting*, Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling, San Francisco, CA, Apr. 2–6, **2017**. Contributed.

Radak, B. K. and Roux, B. Assessing and Optimizing Efficiency in Nonequilibrium Molecular Dynamics/Monte Carlo Simulations, *ACS 253rd National Meeting*, Molecular Mechanics: Protons & Electrons, San Francisco, CA, Apr. 2–6, **2017**. Contributed.

Radak, B. K. and Roux, B. Rapid Protocol for Free Energy Calculations via Multidimensional Expanded Ensemble Simulations, *ACS 253rd National Meeting*, Molecular Mechanics: Sampling Long Time Scales, San Francisco, CA, Apr. 2–6, **2017**. Contributed.

Radak, B. K. Towards a neMD/MC Constant pH Method in NAMD, *NAMD Developer Workshop*, Chicago, IL, May **2016**. Invited.

Radak, B. K.; Singharoy, A.; Schulten, K.; Roux, B. Inclusion of pH Effects in Molecular Dynamics Simulations of Membranes and Membrane Proteins, *BPS 60th Annual Meeting*, Los Angeles, CA, Feb. 27–Mar. 2, **2016**; Poster.

Radak, B. K. Detours and Discoveries While Implementing a Constant pH Simulation Method in NAMD, *University of Illinois, Urbana-Champaign Theoretical and Computational Biophysics Group Seminar*, Urbana, IL, July 27, **2015**; Invited.

Radak, B. K. Implementation of a Constant pH Simulation Method in NAMD *5th Annual Meeting of the Membrane Protein Structure Dynamics Consortium*, Chicago, IL, Apr. 29–May 1, **2015**; Invited.

Radak, B. K. Multiscale Molecular Simulations of RNA Catalysis, *NIH Computational Biophysics Section Seminar*, Rockville, MD, Sept. 4, **2014**; Invited.

Radak, B. K.; Lee, T.; York, D. M. Exploring RNA catalysis in the Hepatitis Delta Virus Ribozyme with QM/MM Simulations: Microscopic Details of General Acid Catalysis, *ACS 245th National Meeting*, Frontiers in RNA Catalysis and Folding: Interface of Theory and Experiment, New Orleans, LA, Apr. 7–19, **2013**; Contributed.

Awards and Honors

Dec 2015 Ruth L. Kirchstein National Research Service Award, NIGMS (Fellowship Declined)

Fall 2012 Peter Kollmann Graduate Award in Supercomputing, ACS Division of Computers in Chemistry and National Institute for Computational Sciences

2008-2009 Graham N. Gleysteen Fellowship in Chemistry, University of Minnesota, Dept. of Chemistry

Teaching Experience

University of Minnesota, Department of Chemistry

2008-2010 Teaching Assistant - Chemical Principles I,II

2009 Teaching Assistant - (Graduate) Quantum Mechanics I

Northwestern University, Integrated Science Program

2007-2008 Instructor - Computing Applications

2006-2007 Teaching Assistant - Computing Applications

Affiliations and Service

Memberships American Chemical Society (**2008-**), Biophysical Society (**2015-**)

Ad Hoc Reviewer ACS Catalysis, Entropy, Journal of Physical Chemistry Letters

Reviewer Computational Readiness, Innovative and Novel Computational Impact on Theory and Experiment (INCITE) (**2016**)