1) Refereed journal articles (partial list)

Bergonzo, C., Hall, K.B., Cheatham, T.E. III. 2016. Divalent Ion Dependent Conformational Changes in an RNA Stem-Loop Observed by Molecular Dynamics. *Journal of Chemical Theory and Computation,* 12, 3382-3389.

Bergonzo, C., Hall, K.B., Cheatham, T.E. III. 2015. Stem-loop V of Varkud Satellite RNA Exhibits Characteristics of the Mg^{2+} Bound Structure in the Presence of Monovalent Ions. *Journal of Physical Chemistry B,* 119, 12355-12364.

Bergonzo, C., Cheatham, T.E. III. 2015. Improved Force Field Parameters Lead to a Better Description of RNA Structure. *Journal of Chemical Theory and Computation*, 11, 3969-3972.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. 2015. Highly sampled tetranucleotide and tetraloop motifs enable evaluation of common RNA force fields. *RNA Journal*, 21, 1578-1590.

Kuznetsov, N.A. and **Bergonzo, C.**, Campbell, A.J., Li, H., Mechetin, G.V., de los Santos, C., Grollman, A.P., Fedorova, O.S., Zharkov, D.O., Simmerling, C. 2014. Active destabilization of base pairs by a DNA glycosylase wedge initiates damage recognition. *Nucleic Acids Research,* 43, 272-281.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Swails, J.M., Roitberg, A.E., Cheatham, T.E. III. 2014. Multi-dimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. *Journal of Chemical Theory and Computation*, 10, 492-499.

Bergonzo, C., Campbell, A.J, de los Santos, C., Grollman, A.P., Simmerling, C. 2011. Energetic Preference of 8-oxoG Eversion Pathways in a DNA Glycosylase. *Journal of the American Chemical Society*, 133, 14504-14506.

2) Book chapters (partial list)

Bergonzo, C., Galindo-Murillo, R., and Cheatham, T.E. III. 2013. Molecular modeling of nucleic acid structure: Energy and Sampling. *Current Protocols Nucleic Acid Chemistry*, 54, 7.8.1-7.8.21.

Bergonzo, C., Galindo-Murillo, R., and Cheatham, T.E. III. 2013. Molecular modeling of nucleic acid structure: Electrostatics and solvation. *Current Protocols Nucleic Acid Chemistry*, 55, 7.9.1-7.9.27.

3) Published proceedings (partial list)

Bergonzo, C., Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. 2014. Overcoming the Sampling Problem in Force Field Evaluation via GPU-accelerated Multi-dimensional Replica Exchange Molecular Dynamics. *Abstracts of papers of the American Chemical Society,* 248.

6) Presentations (partial list)

Bergonzo, C., Cheatham, T.E. III. 2016. "Computational RNA Dynamics: The Good, the Bad, and the Ugly." Oral Presentation, Department of Medicinal Chemistry, College of Pharmacy, University of Utah, UT.

Bergonzo, C. 2015. "Nucleic Acids Through a Virtual Microscope: The Potential and Promise of Simulation." Invited Talk, The Ohio State University, OH.

Bergonzo, C., Henriksen, N.M., Roe, D.R., Cheatham, T.E. III. 2014. "Evaluating Force Field Accuracy of RNA Dynamics Using Enhanced Sampling Methods." Oral Presentation, American Chemical Society 248th National Meeting, San Francisco, CA.

Bergonzo, C., and Cheatham, T.E. III. 2014. "Evaluating Nucleic Acid Force Fields using Multi-dimensional Replica Exchange." Oral Presentation, International Society of Quantum Biology and Pharmacology President's Meeting, Telluride, CO.