Tyler Luchko

Department of Physics and Astronomy
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Education

Ph.D.	Molecular modeling of protein-protein/protein solvent interactions, focusing on microtubules and statistical mechanical molecular solvation theory. Department of Physics, University of Alberta, Canada. National Institute for Nanotechnology, National Research Council, Canada. Advisors: Dr. Jack Tuszynski and Dr. Andriy Kovalenko	11/20/2008
B.Sc.	Specialization Physics. University of Alberta, Canada.	2000

Research Interests

Development of solvation theory and molecular modeling methods with applications to molecular biology and computer-aided drug discovery and design.

Current Position

Associate Professor	Department of Physics and Astronomy California State University, Northridge	08/2019-Present

Research Experience

Assistant Professor	Department of Physics and Astronomy California State University, Northridge	08/2013-07/2019
Postdoctoral Associate	BioMaPS Institute, Rutgers University, USA Advisor: Dr. David A. Case	05/2009-08/2013
Postdoctoral Fellow	Department of Mechanical Engineering, University of Alberta, Canada National Institute for Nanotechnology, National Research Council, Canada Advisor: Dr. Andriy Kovalenko	09/2008-04/2009
Postdoctoral Fellow	Department of Oncology, University of Alberta, Canada Advisor: Dr. Jack Tuszynski	05/2008-08/2008

Current Funding

Principle Investigator	National Science Foundation #2102668	07/01/2021-06/30/2024
Co-Principle Investigator	Research Corporation for Science Advancement Cottrell Collaborative Award	10/01/2019-10/01/2022

Awards

	Cottrell Scholar Award Research Corporation for the Advancement of Science	07/2017-12/2020

Postgraduate Scholarship D Natural Science and Engineering Research Council of Canada	05/2006-04/2008
Walter H. Johns Fellowship University of Alberta	09/2006-04/2008
National Research Council Canada Graduate Student Scholarship Supplement Program National Institute for Nanotechnology	09/2005-06/2008
Province of Alberta Graduate Fellowship University of Alberta	05/2005-04/2006
Province of Alberta Graduate Scholarship University of Alberta, Canada	09/2002-04/2003
Graduate Summer Scholarship Province of Alberta	04/2002
NSERC Undergraduate Student Research Award Simon Fraser University	05/2000-08/2000
JA Jacobs Prize in Physics University of Alberta	05/2000
University of Alberta Merit-Based Bursary University of Alberta	03/2000

Refereed Publications

[24]Wilson, L., Krasny, R., and **Luchko, T. 2022**, "Accelerating the 3D reference interaction site model theory of molecular solvation with treecode summation and cut-offs," Journal of Computational Chemistry **43**, 1251–1270 10.1002/jcc.26889.

[23]Gray, J. G., Giambaşu, G. M., Case, D. A., and **Luchko, T. 2022**, "Integral equation models for solvent in macromolecular crystals," The Journal of Chemical Physics **156**, Publisher: American Institute of Physics, 014801 10.1063/5.0070869.

[22]Greene, D., **Barton, M.**, **Luchko, T.**, and Shiferaw, Y. **2021**, "Computational Analysis of Binding Interactions between the Ryanodine Receptor Type 2 and Calmodulin," The Journal of Physical Chemistry B **125**, Publisher: American Chemical Society, 10720–10735 10.1021/acs.jpcb.1c03896.

[21]Olson, B., Cruz, A., Chen, L., Ghattas, M., Ji, Y., Huang, K., **Ayoub, S.**, **Luchko, T.**, McKay, D. J., and Kurtzman, T. **2020**, "An online repository of solvation thermodynamic and structural maps of SARS-CoV-2 targets," Journal of Computer-Aided Molecular Design **34**, 1219–1228 10.1007/s10822-020-00341-x.

[20]**McMillin, P. J.**, **Alegrete, M.**, Peric, M., and **Luchko, T. 2020**, "Electron paramagnetic resonance measurements of four nitroxide probes in supercooled water explained by molecular dynamics simulations," The Journal of Physical Chemistry B **124**, 3962–3972 10.1021/acs.jpcb.0c00684.

[19]Nguyen, C., Yamazaki, T., Kovalenko, A., Case, D. A., Gilson, M. K., Kurtzman, T., and **Luchko, T. 2019**, "A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site," eng, PloS One **14**, e0219473 10.1371/journal.pone.0219473.

[18]**Tsednee, T.** and **Luchko, T. 2019**, "Closure for the Ornstein-Zernike equation with pressure and free energy consistency," Physical Review E **99**, 032130 10.1103/PhysRevE.99.032130.

[17]**Luchko, T.**, Blinov, N., Limon, G., Joyce, K., and Kovalenko, A. **2016**, "SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling," Journal of Computer-Aided Molecular Design, 1–13 10.1007/s10822-016-9947-7.

[16]Johnson, J., Case, D. A., Yamazaki, T., Gusarov, S., Kovalenko, A., and **Luchko, T. 2016**, "Small molecule hydration energy and entropy from 3d-RISM," Journal of Physics: Condensed Matter **28**, 344002 10.1088/0953-8984/28/34/344002.

[15]Giambaşu, G. M., Gebala, M. K., Panteva, M. T., **Luchko, T.**, Case, D. A., and York, D. M. **2015**, "Competitive interaction of monovalent cations with DNA from 3D-RISM," Nucleic Acids Research, gkv830 10.1093/nar/gkv830.

[14]Giambaşu*, G. M., Luchko*, T., Herschlag, D., York, D. M., and Case, D. A. **2014**, "Ion counting from explicit-solvent simulations and 3D-RISM," Biophysical Journal **106**, (* contributed equally.), 883–894 10.1016/j.bpj.2014.01.021.

[13]Joung, I. S., **Luchko, T.**, and Case, D. A. **2013**, "Simple electrolyte solutions: comparison of DRISM and molecular dynamics results for alkali halide solutions," J Chem Phys **138**, 044103 doi:10.1063/1.4775743.

[12]**Luchko, T.** and Case, D. **2012**, "Implicit solvent models and electrostatics in molecular recognition," in Protein-ligand interactions, edited by H. Gohlke (Wiley-VCH Verlag GmbH & Co. KGaA), pp. 171–189, 10.1002/9783527645947.ch9/summary.

[11]**Luchko, T.**, Joung, I. S., and Case, D. A. **2012**, "Integral equation theory of biomolecules and electrolytes," in Innovations in biomolecular modeling and simulation, edited by T. Schlick (Royal Society of Chemistry), pp. 51–86, 10.1039/9781849735049-00051.

[10]Freedman, H., **Luchko, T.**, Luduena, R. F., and Tuszynski, J. A. **2011**, "Molecular dynamics modeling of tubulin C-terminal tail interactions with the microtubule surface," Proteins **79**, 2968–2982 10.1002/prot.23155.

[9]Genheden, S., **Luchko, T.**, Gusarov, S., Kovalenko, A., and Ryde, U. **2010**, "An MM/3D-RISM approach for ligand binding affinities," English, J Phys Chem B **114**, 8505–8516 10.1021/jp101461s.

[8]**Luchko, T.**, Gusarov, S., Roe, D. R., Simmerling, C., Case, D. A., Tuszynski, J., and Kovalenko, A. **2010**, "Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber," English, J Chem Theory Comput **6**, 607–624 10.1021/ct900460m.

[7]Barakat, K. H., Huzil, J. T., **Luchko, T.**, Jordheim, L., Dumontet, C., and Tuszynski, J. **2009**, "Characterization of an inhibitory dynamic pharmacophore for the ERCC1-XPA interaction using a combined molecular dynamics and virtual screening approach," J Mol Graph Model **28**, 113–130 10.1016/j.jmgm.2009.04.009.

[6]Bennett, M. J., Chik, J. K., Slysz, G., **Luchko, T.**, Tuszynski, J., Sackett, D. L., and Schriemer, D. C. **2009**, "Structural mass spectrometry of the $\alpha\beta$-tubulin dimer supports a revised model of microtubule assembly.," Biochemistry **48**, 4858–4870 10.1021/bi900200q.

[5]**Luchko, T.**, Huzil, J., Stepanova, M., and Tuszynski, J. **2008**, "Conformational analysis of the carboxy-terminal tails of human β-tubulin isotypes," Biophys J **94**, 1971–1982 10.1529/biophysj.107.115113.

[4]Freedman, H., Huzil, T., **Luchko, T.**, Luduena, R., and Tuszynski, J. A. **2008**, "Identification and characterization of an intermediate taxol binding site within microtubule nanopores and a mechanism for tubulin isotype binding selectivity," J Chem Inf Model **49**, 424–436 10.1021/ci8003336.

[3]Tuszynski, J. A., Carpenter, E. J., Huzil, J. T., Malinski, W., **Luchko, T.**, and Luduena, R. F. **2006**, "The evolution of the structure of tubulin isoforms and its potential consequences for the role and function of microtubules in cells and embryos," Int J Dev Biol **50**, 341–58 10.1387/ijdb.052063jt.

[2]Tuszynski, J. A., **Luchko, T.**, Portet, S., and Dixon, J. M. **2005**, "Anisotropic elastic properties of microtubules," Eur Phys J E Soft Matter **17**, 29–35 10.1140/epje/i2004-10102-5.

[1]Tuszynski, J. A., **Luchko, T.**, Carpenter, E. J., and Crawford, E. **2004**, "Results of molecular dynamics computations of the structural and electrostatic properties of tubulin and their consequences for microtubules," J Comput Theor Nanosci **1**, 392–397 10.1166/jctn.2004.042.

Invited Presentations

[18]**Luchko, T. 2021**, Faster, more accurate 3d-rism from improved solvers and thermodynamically consistent closures, (Invited talk), Honolulu, Hawaii, USA: Pacifichem 2021 International Chemical Congress of Pacific Basin Socities.

[17]Wilson, L., **Limon, G. C.**, Kransy, R., and **Luchko, T. 2018**, Accelerating the 3D-RISM implicit solvent model using treecode and multigrid methods, (Invited Talk), Portland, OR, USA: 2018 SIAM Annual Meeting.

[16]Wilson, L., **Limon, G. C.**, Kransy, R., and **Luchko, T. 2018**, Accelerating the 3D-RISM implicit solvent model using treecode and multigrid methods, (Invited Talk), Edmonton, Alberta, Canada: Canadian Chemistry Conference.

[15]**Luchko, T. 2017**, Decomposing the solvent environment of biomolecules using 3D-RISM, (Invited talk), California State University, Los Angeles, Los Angeles, USA: Department of Physics and Astronomy Colloquium.

[14]**Joyce, K. P.** and **Luchko, T. 2017**, Progress towards rigorous drug-binding predictions from 3D-RISM, (Invited talk), California State University, Northridge, California, USA: 7th Annual Interdisciplinary Research Institute for the Sciences Symposium.

[13]**Luchko, T. 2017**, Understanding the solvent environment of biomolecules using 3d-rism, (Invited talk), Irvine, California, USA: SoCal TheoChem 2.0.

[12]**Luchko, T. 2016**, Breaking down hydration on the molecular scale, (Invited talk), California State University, Northridge, California, USA: 6th Annual Interdisciplinary Research Institute for the Sciences Symposium.

[11]**Luchko, T. 2016**, Solvation free energy decomposition using the 3d-rism theory of molecular solvation, (Invited talk), Pittsburgh, Pennsylvania, USA: 252nd American Chemical Society National Meeting & Exposition.

[10]**Luchko, T. 2016**, Solvation free energy decomposition using the 3d-rism theory of molecular solvation, (Invited talk), Boston, Massachusetts, USA: 2016 SIAM Conference on the Life Sciences.

[9]**Luchko, T. 2015**, DNA, drug design and salty water - three tales of modeling with 3D-RISM, (Invited talk), California State University, Northridge, California, USA: Interdisciplinary Research Institute for the Sciences Seminar Series.

[8]**Luchko, T. 2015**, High accuracy solvation enthalpies, entropies, and free energies from 3D-RISM, (Invited talk), Honolulu, Hawaii, USA: Pacifichem 2015 International Chemical Congress of Pacific Basin Socities.

[7]**Luchko, T. 2015**, Modeling complex liquids around biomolecules, (Invited talk), California State University, Northridge, California, USA: 5th Annual Interdisciplinary Research Institute for the Sciences Symposium.

[6]**Luchko, T. 2015**, Modeling water around biomolecules with the integral equation theory of molecular solvation, (Invited talk), California State University, Northridge, California, USA: Department of Mathematics Applied Mathematics Seminar.

[5]**Luchko, T. 2014**, The ionic atmosphere of DNA, (Invited talk), California State University, Long Beach, Long Beach, California, USA: Department of Chemistry & Biochemistry Allergan Foundation Seminar Series.

[4]**Luchko, T.**, Giamasu, G. M., Cai, Q., Luo, R., York, D. M., and Case, D. A. **2013**, DNA structure and solvation calculated with the 3D-RISM molecular theory of solvation, (Invited talk), Indianapolis, Indiana, USA: 246th American Chemical Society National Meeting & Exposition.

[3]**Luchko, T.**, Nguyen, C., Case, D. A., Gilson, M. K., and Kurtzman, T. **2013**, Protein-ligand binding solvation thermodynamics from 3D-RISM, (Invited poster), Napa, California, USA: Current Challenges in Computing 2013.

[2]**Luchko, T. 2013**, Quantitative calculations of the ionic atmosphere of DNA, (Invited talk), University of California, Irvine, Irvine, California, USA: Computational Biology Seminar Series.

[1]**Luchko, T. 2012**, Calculation of the ionic atmosphere of DNA using 3D-RISM and molecular dynamics, (Invited talk), Lehman College, Bronx, NY.

Current Group Members

Master's	Vahe Grigorian (former undergraduate)	01/2021 – Present
Undergraduate	Alexander McMahon	09/2020 – Present
Master's	Sean Reilly	08/2020 – Present
Master's	Dylan Daw	09/2019 – Present
Master's	Tiannah York Van Elselande (former undergraduate)	05/2019 – Present
Master's	Steven Ayoub (former undergraduate)	01/2018 – Present
Volunteer	Michael Barton (former undergraduate and graduate)	11/2017 – Present

Former Group Members

Research Assistant	Ezequiel Donovan (former undergraduate)	09/2020 – 09/2021
Postdoctoral Scholar	Tsogbayar Tsednee	06/2017 – 08/2020
Undergraduate	Lizet Casillas, masters student at CSUN	05/2017 – 08/2019
High School	Sifath Mannan, undergraduate student at University of California, Berkeley	06/2017 – 08/2018
Master's and Undergraduate	Garrett Limon, PhD Student at Univeristy of Michigan, National Science Foundation Graduate Fellow	02/2015 – 08/2018
Undergraduate	Patrick McMillin, PhD student at University of California, Los Angeles	06/2016 – 08/2018
Undergraduate	Kevin Joyce	04/2015 – 10/2017
Undergraduate	Matthew Alegrete	01/2014 – 06/2015
Undergraduate	Jacob Kleine	11/2013 – 02/2015

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