Tyler Luchko

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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	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

Teaching

PHYS 497	Senior Project Reseach project and methods. 13-18 students.	2021-2023
PHYS 490	Computer Applications in Physics Upper division computational physics and numerical methods. 6-9 students.	2014-2016

PHYS 431	Thermodynamics and Statistical Mechanics Upper division thermodynamics and statistical mechanics of weakly interacting classical and quantum systems. 9-11 students.	2013-2014
PHYS 365	Experimental Physics I Introduction to computational physics. 17-19 students.	2017-2019
PHYS 227	Physics III (Thermal and Modern Physics) Introduction to thermodynamics, relativity, quantum mechanics, atomic physics and particle physics, primarily for physics and astronomy students. 15-20 students.	2015-2017
PHYS 100B	General Physics II (Electromagnetism, Optics, and Modern Physics) Introduction to electricity, magentism, geometric optics, quantum mechanics, atomic physics, and nuclear physics primarily for life-sciences students. 49-120 students.	2018-2022

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	10/01/2022-10/01/2024
Sponsor	Research Corporation for Science Advancement Cottrell Postbac Award	09/01/2023-08/31/2024

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

[28] Casillas, Lizet, Grigorian, Vahe M., and Luchko, Tyler. **2023**. "Identifying Systematic Force Field Errors Using a 3D-RISM Element Counting Correction." In: Molecules 28.3, p. 925. doi: 10.3390/molecules28030925.

[27] Gray, Jonathon G., Giambaşu, George M., Case, David A., and Luchko, Tyler. **2022**. "Integral equation models for solvent in macromolecular crystals." In: The Journal of Chemical Physics 156.1, p. 014801. doi: 10.1063/5.0070869.

[26] Greene, D'Artagnan, Barton, Michael, Luchko, Tyler, and Shiferaw, Yohannes. **2022**. "Molecular Dynamics Simulations of the Cardiac Ryanodine Receptor2 Type 2 (RyR2) Gating Mechanism." In: Journal of Physical Chemistry B 126.47, pp. 9790–9809. doi: 10.1021/acs.jpcb.2c03031.

[25] Greene, D'Artagnan, Luchko, Tyler, and Shiferaw, Yohannes. **2022**. "The role of subunit cooperativity on ryanodine receptor 2 calcium signaling." In: Biophysical Journal. doi: 10.1016/j.bpj.2022.11.008. (In press.)

[24] Wilson, Leighton, Krasny, Robert, and Luchko, Tyler. **2022**. "Accelerating the 3D reference interaction site model theory of molecular solvation with treecode summation and cut-offs." In: Journal of Computational Chemistry 43.18, pp. 1251–1270. doi: 10.1002/jcc.26889.

[23] Greene, D'Artagnan, Barton, Michael, Luchko, Tyler, and Shiferaw, Yohannes. **2021**. "Computational Analysis of Binding Interactions between the Ryanodine Receptor Type 2 and Calmodulin." In: The Journal of Physical Chemistry B 125.38. Publisher: American Chemical Society, pp. 10720–10735. doi: 10.1021/acs.jpcb.1c03896.

[22] McMillin, Patrick J., Alegrete, Matthew, Peric, Miroslav, and Luchko, Tyler. **2020**. "Electron paramagnetic resonance measurements of four nitroxide probes in supercooled water explained by molecular dynamics simulations." In: The Journal of Physical Chemistry B 124.19, pp. 3962–3972. doi: 10.1021/acs.jpcb.0c00684.

[21] Olson, Brian, Cruz, Anthony, Chen, Lieyang, Ghattas, Mossa, Ji, Yeonji, Huang, Kunhui, Ayoub, Steven, Luchko, Tyler, McKay, Daniel J., and Kurtzman, Tom. **2020**. "An online repository of solvation thermodynamic and structural maps of SARS-CoV-2 targets." In: Journal of Computer-Aided Molecular Design 34.12, pp. 1219–1228. doi: 10.1007/s10822-020-00341-x.

[20] Nguyen, Crystal, Yamazaki, Takeshi, Kovalenko, Andriy, Case, David A., Gilson, Michael K., Kurtzman, Tom, and Luchko, Tyler. **2019**. "A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site." In: PloS One 14.7, e0219473. doi: 10.1371/journal.pone.0219473.

[19] Tsednee, Tsogbayar and Luchko, Tyler. **2019**. "Closure for the Ornstein-Zernike equation with pressure and free energy consistency." In: Physical Review E 99.3, p. 032130. doi: 10.1103/PhysRevE.99.032130.

[18] Johnson, J., Case, D. A., Yamazaki, T., Gusarov, S., Kovalenko, A., and Luchko, T. **2016**. "Small molecule hydration energy and entropy from 3D-RISM." In: Journal of Physics: Condensed Matter 28.34, p. 344002. doi: 10.1088/0953-8984/28/34/344002.

[17] Luchko, T., Blinov, Nikolay, Limon, Garrett C., Joyce, Kevin P., and Kovalenko, Andriy. **2016**. "SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling." In: Journal of Computer-Aided Molecular Design, pp. 1–13. doi: 10.1007/s10822-016-9947-7.

[16] Giambaşu, George M., Gebala, Magdalena K., Panteva, Maria T., Luchko, T., Case, David A., and York, Darrin M. **2015**. "Competitive interaction of monovalent cations with DNA from 3D-RISM." In: Nucleic Acids Research, gkv830. doi: 10.1093/nar/gkv830.

[15] Giambaşu*, George M., Luchko*, T., Herschlag, Daniel, York, Darrin M., and Case, David A. **2014**. "Ion counting from explicit-solvent simulations and 3D-RISM." In: Biophysical Journal 106.4. (* contributed equally.), pp. 883–894. doi: 10.1016/j.bpj.2014.01.021.

[14] Joung, In Suk, Luchko, T., and Case, David A. **2013**. "Simple electrolyte solutions: Comparison of DRISM and molecular dynamics results for alkali halide solutions." In: J Chem Phys 138, p. 044103. doi: doi:10.1063/1.4775743.

[13] Luchko, T. and Case, D. A. **2012**. "Implicit Solvent Models and Electrostatics in Molecular Recognition." In: Protein-Ligand Interactions. Ed. by Holger Gohlke. Wiley-VCH Verlag GmbH & Co. KGaA, pp. 171–189. doi: 10.1002/9783527645947.ch9/summary.
[12] Luchko, T., Joung, I. S., and Case, David A. **2012**. "Integral Equation Theory of Biomolecules and Electrolytes." In: Innovations in Biomolecular Modeling and Simulation. Ed. by Tamar Schlick. Royal Society of Chemistry, pp. 51–86. doi: 10.1039/9781849735049-00051.
[11] Freedman, Holly, Luchko, T., Luduena, Richard F., and Tuszynski, Jack A. **2011**. "Molecular dynamics modeling of tubulin C-terminal tail interactions with the microtubule surface." In: Proteins 79.10, pp. 2968–2982. doi: 10.1002/prot.23155.
[10] Genheden, Samuel, Luchko, T., Gusarov, Sergey, Kovalenko, Andriy, and Ryde, Ulf. **2010**. "An MM/3D-RISM approach for ligand binding affinities." In: J Phys Chem B 114.25, pp. 8505–8516. doi: 10.1021/jp101461s.
[9] Luchko, T., Gusarov, Sergey, Roe, Daniel R., Simmerling, Carlos, Case, David A., Tuszynski, Jack, and Kovalenko, Andriy. **2010**. "Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber." In: J Chem Theory Comput 6.3, pp. 607–624. doi: 10.1021/ct900460m.
[8] 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." In: J Mol Graph Model 28 (2), pp. 113–130. doi: 10.1016/j.jmgm.2009.04.009.
[7] Bennett, M. J., Chik, J. K., Slysz, G. W., 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." In: Biochemistry 48 (22), pp. 4858–4870. doi: 10.1021/bi900200q.
[6] Freedman, Holly, Huzil, Torin, Luchko, T., Luduena, Richard, and Tuszynski, Jack A. **2008**. "Identification and characterization of an intermediate taxol binding site within microtubule nanopores and a mechanism for tubulin isotype binding selectivity." In: J Chem Inf Model 49 (2), pp. 424–436. doi: 10.1021/ci8003336.
[5] Luchko, T., Huzil, J. T., Stepanova, M., and Tuszynski, J. **2008**. "Conformational analysis of the carboxy-terminal tails of human β-tubulin isotypes." In: Biophys J 94, pp. 1971–1982. doi: 10.1529/biophysj.107.115113.
[4] Tuszyński, J. A., Malinski, W., Carpenter, E. J., Luchko, T., Torin Huzil, J., and Ludeña, R. F. **2008**. "Tubulin electrostatics and isotype specific drug binding." In: Canadian Journal of Physics 86.4, pp. 635–640. doi: 10.1139/p07-199.
[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." In: Int J Dev Biol 50, pp. 341–58. doi: 10.1387/ijdb.052063jt.
[2] Tuszynski, J. A., Luchko, T., Portet, S., and Dixon, J. M. **2005**. "Anisotropic elastic properties of microtubules." In: Eur Phys J E Soft Matter 17.1, pp. 29–35. doi: 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." In: J Comput Theor Nanosci 1.4, pp. 392–397. doi: 10.1166/jctn.2004.042.

Invited Presentations

[20] Luchko, T. **2022**. Big, small and periodic: increasing the application-space of molecular solvation theory with treecodes, cutoffs and Ewald. (Invited talk). Pittsburgh, Pennsylvania, USA: 2022 SIAM Conference on the Life Sciences.
[19] 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.
[18] Wilson, Leighton, Limon, Garrett C., Kransy, Robert, 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.

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

[16] Joyce, Kevin 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.

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

[13] 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.

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

[11] 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.

[10] 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.

[9] 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.

[8] 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.

[7] 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.

[6] Luchko, T. **2015**. Partial Molar Volume Corrected Solvation Energies, Entropies and Free Energies from 3D-RISM. (Invited talk). University of Ohio, Columbus, Ohio: Mathematical Biosciences Institute Multiple Faces of Biomolecular Electrostatics.

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

[3] Luchko, T., Giamasu, George M., Cai, Qin, Luo, Ray, York, Darrin M., and Case, David 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.

[2] Luchko, Tyler, Nguyen, Crystal, Case, David A., Gilson, Michael K., and Kurtzman, Thomas. **2013**. Protein-Ligand Binding Solvation Thermodynamics from 3D-RISM. (Invited poster). Napa, California, USA: Current Challenges in Computing 2013.

[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

Undergraduate	Noah Pishaki	06/2022 – Present
Master's & Undergraduate	Vahe Grigorian	11/2020 – Present

Undergraduate	Alexander McMahon	09/2020 – Present
Master's	Dylan Daw	09/2019 – Present
Master's & Undergraduate	Tiannah York Van Elselande	06/2019 – Present
Master's & Undergraduate	Steven Ayoub	01/2018 – Present
Volunteer & Master's & Undergraduate	Michael Barton	11/2017 – Present

Former Group Members

Master's	Sean Reilly	08/2020 – 07/2022
Research Assistant & Undergraduate	Ezequiel Donovan	09/2020 – 09/2021
Postdoctoral Scholar	Tsogbayar Tsednee (Postdoctoral Scholar at University of North Dakota)	06/2017 – 08/2020
Undergraduate	Lizet Casillas (PhD student at UCLA)	05/2017 – 08/2019
High School	Sifath Mannan (undergraduate student at UC Berkeley)	06/2017 – 08/2018
Master's & Undergraduate	Garrett Limon (PhD Student at Univeristy of Michigan)	02/2015 – 08/2018
Undergraduate	Patrick McMillin, (PhD student at UCLA)	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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