

# Tyler Luchko

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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.<br>Department of Physics, University of Alberta, Canada.<br>National Institute for Nanotechnology, National Research Council, Canada.<br>Advisors: Dr. Jack Tuszynski and Dr. Andriy Kovalenko | 2008 |
| B.Sc. | Specialization Physics.<br>University of Alberta, Canada.  | 2000 |

## Current Position

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

## Research Experience

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

## Current Funding

|                        |   |                           |
|------------------------|---|---------------------------|
| Principle Investigator | 2020 Research and Sponsored Programs Summer Grant Program<br>Fast GPU-based 3D-RISM for drug-discovery and design   | 06/01/2020–<br>08/20/2020 |
| Principle Investigator | 2020-21 Competition for Research, Scholarship and Creative Activity Awards<br>Modeling liquids with machine learning from fundamental physics to drug discovery | 07/01/2020–<br>06/30/2021 |
| Principle Investigator | Extreme Science and Engineering Discovery Environment (XSEDE) Research Allocation #TG-MCB190048   | 07/01/2019-06/30/2020     |
| Principle Investigator | Research Corporation for Science Advancement Cottrell Scholar Award #23967  | 07/15/2017-06/30/2020     |
| Principle Investigator | National Science Foundation Grant #1566638  | 07/15/2016-06/30/2020     |

## Pending Proposals

## Past Funding

|                        |  |                       |
|------------------------|--|-----------------------|
| Principle Investigator | Extreme Science and Engineering Discovery Environment (XSEDE) Startup Allocation #TG-MCB170153 | 11/05/2017-08/05/2019 |
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| Principle Investigator | California State University Program for Education and Research in Biotechnology (CSUPERB) New Investigator Grant | 06/01/2015-11/30/2016 |
| Principle Investigator | Spring 2015: Probationary Faculty Support Program  | 01/20/2015-05/30/2015 |
| Principle Investigator | 2014-15 Competition for Research, Scholarship and Creative Activity Awards                                       | 08/20/2014-12/30/2014 |
| Principle Investigator | Spring 2014: Probationary Faculty Support Program  | 01/20/2014-05/30/2014 |

## Refereed Publications

Names of group members are in bold.

- [20] McMillin, P. J.; **Alegrete, M.**; Peric, M.; **Luchko, T.** Electron Paramagnetic Resonance Measurements of Four Nitroxide Probes in Supercooled Water Explained by Molecular Dynamics Simulations. *The Journal of Physical Chemistry B* **2020**, 124, Publisher: American Chemical Society, 3962–3972.
- [19] **Tsednee, T.**; **Luchko, T.** Closure for the Ornstein-Zernike equation with pressure and free energy consistency. *Physical Review E* **2019**, 99, 032130.
- [18] Nguyen, C.; Yamazaki, T.; Kovalenko, A.; Case, D. A.; Gilson, M. K.; Kurtzman, T.; **Luchko, T.** Comparing 3D-RISM and GIST hydration thermodynamic maps in an enzyme active site. **2019**, (Under revision.)
- [17] **Luchko, T.**; Blinov, N.; **G.C. Limon**; **K.P. Joyce**; Kovalenko, A. SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. *Journal of Computer-Aided Molecular Design* **2016**, 1–13.
- [16] Johnson, J.; Case, D. A.; Yamazaki, T.; Gusarov, S.; Kovalenko, A.; **Luchko, T.** Small molecule hydration energy and entropy from 3D-RISM. *Journal of Physics: Condensed Matter* **2016**, 28, 344002.
- [15] Giambaşu, G. M.; Gebala, M. K.; Panteva, M. T.; **Luchko, T.**; Case, D. A.; York, D. M. Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research* **2015**, gkv830.
- [14] Giambaşu\*, G. M.; **Luchko\***, T.; Herschlag, D.; York, D. M.; Case, D. A. Ion Counting from Explicit-Solvent Simulations and 3D-RISM. *Biophysical Journal* **2014**, 106, (\* contributed equally.), 883–894.
- [13] Joung, I. S.; **Luchko, T.**; Case, D. A. Simple electrolyte solutions: Comparison of DRISM and molecular dynamics results for alkali halide solutions. *J Chem Phys* **2013**, 138, 044103.
- [12] **Luchko, T.**; Joung, I. S.; Case, D. A. In *Innovations in Biomolecular Modeling and Simulation*, Schlick, T., Ed.; Royal Society of Chemistry: 2012, pp 51–86.
- [11] **Luchko, T.**; Case, D. In *Protein-Ligand Interactions*, Gohlke, H., Ed.; Wiley-VCH Verlag GmbH & Co. KGaA: 2012, pp 171–189.
- [10] Freedman, H.; **Luchko, T.**; Luduena, R. F.; Tuszynski, J. A. Molecular dynamics modeling of tubulin C-terminal tail interactions with the microtubule surface. *Proteins* **2011**, 79, 2968–2982.
- [9] **Luchko, T.**; Gusarov, S.; Roe, D. R.; Simmerling, C.; Case, D. A.; Tuszynski, J.; Kovalenko, A. Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. *J Chem Theory Comput* **2010**, 6, 607–624.
- [8] Genheden, S.; **Luchko, T.**; Gusarov, S.; Kovalenko, A.; Ryde, U. An MM/3D-RISM Approach for Ligand Binding Affinities. *J Phys Chem B* **2010**, 114, 8505–8516.
- [7] Barakat, K. H.; Huzil, J. T.; **Luchko, T.**; Jordheim, L.; Dumontet, C.; Tuszynski, J. Characterization of an inhibitory dynamic pharmacophore for the ERCC1-XPA interaction using a combined molecular dynamics and virtual screening approach. *J Mol Graph Model* **2009**, 28, 113–130.
- [6] Freedman, H.; Huzil, T.; **Luchko, T.**; Luduena, R.; Tuszynski, J. A. Identification and Characterization of an Intermediate Taxol Binding Site Within Microtubule Nanopores and a Mechanism for Tubulin Isoform Binding Selectivity. *J Chem Inf Model* **2008**, 49, 424–436.

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- [5] Bennett, M. J.; Chik, J. K.; Slysz, G.; **Luchko, T.**; Tuszynski, J.; Sackett, D. L.; Schriemer, D. C. Structural mass spectrometry of the  $\alpha\beta$ -tubulin dimer supports a revised model of microtubule assembly. *Biochemistry* **2009**, 48, 4858–4870.
- [4] **Luchko, T.**; Huzil, J.; Stepanova, M.; Tuszynski, J. Conformational analysis of the carboxy-terminal tails of human  $\beta$ -tubulin isotypes. *Biophys J* **2008**, 94, 1971–1982.
- [3] Tuszynski, J. A.; Carpenter, E. J.; Huzil, J. T.; Malinski, W.; **Luchko, T.**; Luduena, R. F. 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* **2006**, 50, 341–58.
- [2] Tuszynski, J. A.; **Luchko, T.**; Portet, S.; Dixon, J. M. Anisotropic elastic properties of microtubules. *Eur Phys J E Soft Matter* **2005**, 17, 29–35.
- [1] Tuszynski, J. A.; **Luchko, T.**; Carpenter, E. J.; Crawford, E. Results of Molecular Dynamics Computations of the Structural and Electrostatic Properties of Tubulin and Their Consequences for Microtubules. *J Comput Theor Nanosci* **2004**, 1, 392–397.

## Invited Presentations

- [17] Wilson, L.; **Limon, G. C.**; Kransy, R.; **Luchko, T.** Accelerating the 3D-RISM implicit solvent model using treecode and multigrid methods., (Invited Talk), Edmonton, Alberta, Canada: Canadian Chemistry Conference, 2018.
- [16] Wilson, L.; **Limon, G. C.**; Kransy, R.; **Luchko, T.** Accelerating the 3D-RISM Implicit Solvent Model using Treecode and Multigrid Methods., (Invited Talk), Portland, OR, USA: 2018 SIAM Annual Meeting, 2018.
- [15] **Joyce, K.**; **Luchko, T.** 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, 2017.
- [14] **Luchko, T.** Understanding the solvent environment of biomolecules using 3D-RISM., (Invited talk), Irvine, California, USA: SoCal TheoChem 2.0, 2017.
- [13] **Luchko, T.** 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, 2017.
- [12] **Luchko, T.** Solvation free energy decomposition using the 3D-RISM theory of molecular solvation., (Invited talk), Pittsburgh, Pennsylvania, USA: 252nd American Chemical Society National Meeting & Exposition, 2016.
- [11] **Luchko, T.** Solvation free energy decomposition using the 3D-RISM theory of molecular solvation., (Invited talk), Boston, Massachusetts, USA: 2016 SIAM Conference on the Life Sciences, 2016.
- [10] **Luchko, T.** Breaking down hydration on the molecular scale., (Invited talk), California State University, Northridge, California, USA: 6th Annual Interdisciplinary Research Institute for the Sciences Symposium, 2016.
- [9] **Luchko, T.** High accuracy solvation enthalpies, entropies, and free energies from 3D-RISM., (Invited talk), Honolulu, Hawaii, USA: Pacificchem 2015 International Chemical Congress of Pacific Basin Societies, 2015.
- [8] **Luchko, T.** 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, 2015.
- [7] **Luchko, T.** Modeling complex liquids around biomolecules., (Invited talk), California State University, Northridge, California, USA: 5th Annual Interdisciplinary Research Institute for the Sciences Symposium, 2015.
- [6] **Luchko, T.** 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, 2015.

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- [5] **Luchko, T.** The ionic atmosphere of DNA., (Invited talk), California State University, Long Beach, Long Beach, California, USA: Department of Chemistry & Biochemistry Allergan Foundation Seminar Series, 2014.
- [4] **Luchko, T.** Quantitative calculations of the ionic atmosphere of DNA., (Invited talk), University of California, Irvine, Irvine, California, USA: Computational Biology Seminar Series, 2013.
- [3] **Luchko, T.;** Nguyen, C.; Case, D. A.; Gilson, M. K.; Kurtzman, T. Protein-Ligand Binding Solvation Thermodynamics from 3D-RISM., (Invited poster), Napa, California, USA: Current Challenges in Computing 2013, 2013.
- [2] **Luchko, T.;** Giamasu, G. M.; Cai, Q.; Luo, R.; York, D. M.; Case, D. A. 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, 2013.
- [1] **Luchko, T.** Calculation of the ionic atmosphere of DNA using 3D-RISM and molecular dynamics., (Invited talk), Lehman College, Bronx, NY, 2012.

## Current Group Members

|                      |                            |                   |
|----------------------|----------------------------|-------------------|
| Masters              | Dylan Daw                  | 09/2019 – Present |
| Undergraduate        | Tiannah York Van Elselande | 05/2019 – Present |
| Undergraduate        | Steven Ayoub               | 01/2018 – Present |
| Masters              | Michael Barton             | 11/2017 – Present |
| Postdoctoral Scholar | Tsogbayar Tsednee          | 06/2017 – Present |

## Former Group Members

|                           |   |                   |
|---------------------------|---|-------------------|
| 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 |
| Masters 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 |

## Professional Memberships

American Chemical Society 2011-Present

May 14, 2020