# Aram Davtyan

CADD Scientist at Atomwise Inc.

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## Research Fields

Discovery and development of novel therapeutics for oncological, immunological and rare diseases.

Study of molecular mechanisms behind neurodegenerative diseases (Alzheimer's and Parkinson's) and cancer.

Modeling of large-scale molecular processes such as protein-facilitated membrane remodeling.

Development of multi-scale modeling methods for multi-component macromolecular systems.

Theoretical investigation of fundamental phenomena such as protein folding and channel-facilitated molecular transport.

## Education

Ph.D., Chemistry, University of Maryland, College Park, USA — 2013

M.S., Chemistry, University of North Carolina at Chapel Hill, USA — 2010

B.A., Physics, Yerevan State University, Armenia — 2007

## Professional Experience

### Scientist, Computer Aided Drug Design (CADD) — 2019 - present

Atomwise, Inc.
Applying artificial intelligence for drug design and discovery.

### Visiting Scholar — 2019 - present

Center for Theoretical Biological Physics, Rice University
Research in protein aggregation and chromosome organization.

### Independent Postdoctoral Fellow — 2017 - 2019

Center for Theoretical Biological Physics, Rice University
Study of protein misfolding and aggregation in the context of diseases like cancer and Alzheimer's.
Investigation of collective dynamics and channel-facilitated molecular transport.

### Postdoctoral Research Scholar — 2013 - 2017

Department of Chemistry, University of Chicago
Advisor: Greg A. Voth
Multi-scale modeling; development and implementation of coarse-grained and mesoscopic simulation methods.
Applications to protein-facilitated membrane remodeling and ATP hydrolysis in actin filaments.

### Summer Research Fellow — Summer, 2013

Department of Chemistry and Biochemistry, University of Maryland, College Park
Advisor: Garegin A. Papoian
Macromolecular coarse-grained modeling; study of protein folding and protein-protein interactions.

### Visiting Scholar — Summer, 2007

Scripps Research Institute, California
Biomedical research in structural biology; study of metal-ligand and metal-protein interactions using PDB database.

### Scientific Software Developer — 2006 - 2008

Molsoft LLC
Participated in development of "ICM" project; computational chemistry and bioinformatics software. Implementation of IUPAC naming of organic molecules.

### Software Engineer — 2003 - 2008

Softmaster LTD
Accounting software development using Visual FoxPro, SQL and Microsoft Word/Excel COM Server technology.

## Publications

- N. Sobhani, D.R. Tardiel-Cyril, **A. Davtyan**, D. Generali, R. Roudi, Y. Li, "CTLA-4 in regulatory T-cells for cancer immunotherapy", *Cancers*, **2021**, *13(6)*, 1440
- D. S. Yang, A. Saeedi, **A. Davtyan**, M. Fathi, M. B. Sherman, M. S. Safari, A. Klindziuk, M. C. Barton, N. Varadarajan, A. B. Kolomeisky, P. G. Vekilov, "Mesoscopic protein-rich clusters host the nucleation of mutant p53 amyloid fibrils", *PNAS,* **2021,** *118(10)*, e2015618118
- W. Lu, C. Bueno, N. P. Schafer, J. Moller, S. Jin, X. Chen, M. Chen, X. Gu, **A. Davtyan**, J. J. de Pablo, P. G. Wolynes, "OpenAWSEM with Open3SPN2: A fast, flexible, and accessible framework for large-scale coarse-grained biomolecular simulations", PLoS Comput. Biol., **2021**, *17(2),* e1008308
- D. Krepel, **A. Davtyan**, N. P. Schafer, P. G. Wolynes, J. N. Onuchic, "Braiding topology and the energy landscape of chromosome organization proteins", *PNAS*, **2020***, 117(3),* 1468-1477
- S. Jin, V. G. Contessoto, M. Chen, N.P. Schafer, W. Lu, X. Chen, C. Bueno, A. Hajitaheri, B. J. Sirovetz, **A. Davtyan**, G. A. Papoian, M. Y. Tsai, P. G. Wolynes, "AWSEM-Suite: a protein structure prediction server based on template-guided, coevolutionary-enhanced optimized folding landscapes", *Nucleic Acids Res.,* **2020***, 48(W1),* W25-W30
- Z. Jarin, F. C. Tsai, **A. Davtyan**, A. J. Pak, P. Bassereau, G. A. Voth, "Unusual organization of I-BAR proteins on tubular and vesicular membranes", *Biophys. J.,* **2019***, 117(3),* 553-562.
- **A. Davtyan**, A. B. Kolomeisky, "Theoretical insights into mechanisms of channel-facilitated molecular transport in the presence of stochastic gating", *J. Chem. Phys.,* **2019***, 150(12),* 124111
- H. H. Katkar, **A. Davtyan**, A. E. P. Durumeric, G. M. Hocky, A. Schramm, M. Enrique, G. A. Voth, "Insights into the cooperative nature of ATP hydrolysis in actin filaments", *Biophys. J.,* **2018***, 115(8), 1589-1602*
- **A. Davtyan**, M. Simunovic, G. A. Voth, "The Mesoscopic Membrane with Proteins Model (MesM-P)", *J. Chem. Phys.,* **2017***, 147,* 044101
- **A. Davtyan,** G. A. Voth, H. C. Andersen, "Dynamic force matching: Construction of dynamical coarse-grained models for simultaneous capturing of translational and rotational diffusion rates", *J. Chem. Phys.*, **2016***, 145,* 224107
- **A. Davtyan**, M. Simunovic, G. A. Voth, "Multiscale simulations of protein facilitated membrane remodeling", *J. Struct. Biol.,* **2016,** *196(1),* 57-63
- **A. Davtyan**, M. Platkov, M. Gruebele, G. A. Papoian, "Stochastic resonance in protein folding dynamics", *ChemPhysChem,* **2016***, 17(9),* 1305-1313
- K. Dave, **A. Davtyan**, M. Platkov, G. A. Papoian, M. Gruebele, "Environmental fluctuations and stochastic resonance in protein folding", *ChemPhysChem,* **2016***, 17(9),* 1341-1348

- **A. Davtyan,** J. F. Dama, G. A. Voth, H. C. Andersen, "Dynamic force matching: A method for constructing dynamical coarse-grained models with realistic time dependence", *J. Chem. Phys.*, **2015**, *142*, 154104
- **A. Davtyan,** J. F. Dama, A. V. Sinitskiy, G. A. Voth, "The Theory of Ultra-Coarse-Graining. 2. Numerical implementation", *J. Chem. Theory Comput.*, **2014**, *10(12)*, 5265-5275
- W. Zheng, N. P. Schafer, **A. Davtyan**, G. A. Papoian, P. G. Wolynes, "Predictive energy landscapes for protein-protein association", *PNAS*, **2012,** *109(47)*, 19244-19249
- **A. Davtyan**, W. Zheng, N. P. Schafer, C. Clementi, P. G. Wolynes, G. A. Papoian, "AWSEM-MD: Protein structure prediction using coarse-grained physical potential and bioinformatically based local structure biasing", *J. Phys. Chem. B.*, **2012**, *116(29)*, 8494-8503

## Work in Progress and Working Papers (selected)

- Y. Xu, N. P. Schafer, K. Knapp, **A. Davtyan**, M. S. Safari, P. G. Vekilov, P. G. Wolynes, "The transition state for the growth of amyloid β fibrils", *(submitted).*
- **A. Davtyan**, M. Y. Tsai, F. Bai, J. N. Onuchic, P. G. Wolynes, "Rational design of drugs against oligomer-mediated neurodegeneration using novel ensemble of oligomer structures of amyloid β", *(working paper).*

## Teaching Experience

Computational Biophysics — Spring 2018

Guest Lecturer, Department of Chemistry, The University of Hawaii at Manoa

Introduction for Computational Biology — Spring 2018

Guest Lecturer, Department of Bioengineering, Rice University

Physical Chemistry Lab — 2009 - 2010

Department of Chemistry, The University of North Carolina at Chapel Hill

General Chemistry Lab — Fall 2008

Department of Chemistry, The University of North Carolina at Chapel Hill

## Awards and Grants

- XSEDE Research Allocation, National Science Foundation, Equivalent to $16700, 2018
- XSEDE Startup Allocation, National Science Foundation, Equivalent to $5800, 2018
- XSEDE Research Allocation, National Science Foundation, Equivalent to $38000, 2013
- Dean's Fellowship, Department of Chemistry and Biochemistry, The University of Maryland, $5000, Fall 2012
- Dean's Summer Fellowship, Department of Chemistry and Biochemistry, The University of Maryland, $5000, 2012
- Best Undergraduate Student Award, Department of Physics, Yerevan State University, Armenia, 2007
- Victor Hambarcumyan Monthly Scholarship (awarded to the top five students), Department of Physics, Yerevan State University, Armenia, 2005 - 2007

## Professional Service

- Referring for the *Journal of Physical Chemistry, International Journal of Molecular Sciences*

- Associate member of F1000 Research, 2016 - 2018
- Mentoring undergraduate students as part of the Frontiers in Science (FIS) Program, CTBP, Rice University, 2018
- Summer outreach presentations for high-school and college students on “Advances in Theoretical Biochemistry”, Yerevan, Armenia, 2013 - 2016

## Selected Conference Presentations

- ACS Spring Meeting, Virtual, April 2021
- 13th Annual Q-bio Conference, San Francisco, California, August 2019
- ACS National Meeting, Orlando, Florida, April 2019
- 64th Annual Meeting of the Biophysical Society, Baltimore, Maryland, March 2019 (poster)
- SIAM Conference on the Life Sciences (LS18), Minneapolis, Minnesota, August 2018 (session chair and presenter)
- Gordon Research Conference, Computational Chemistry, West Dover, Vermont, July 2018 (poster)
- Gordon Research Seminar, Computational Chemistry, West Dover, Vermont, July 2018 (poster)
- 12th Annual Q-bio Conference, Houston, Texas, June 2018
- 255th ACS National Meeting, New Orleans, Louisiana, March 2018
- The APS March Meeting, Los Angeles, California, March 2018
- Theory and Applications of Computational Chemistry (TACC) Conference, August 2016 (poster)
- SIAM MS16 Conference, Philadelphia, Pennsylvania, May 2016
- XSEDE15 Annual Conference, St. Louis, Missouri, July 2015 (poster)
- The 46th Midwest Theoretical Chemistry Conference (MWTCC), Northwestern University, Evanston, IL, June 2014
- Physics of Living Systems Student Research Network & Sackler Symposium, Yale University, New Haven, Connecticut, July 2012
- The APS March Meeting, Boston, Massachusetts, 2012
- Gordon Research Conference, Protein Folding Dynamics, Ventura, California, January 2012 (poster)
- Gordon Research Seminar, Protein Folding Dynamics, Ventura, California, January 2012 (poster)
- An International Symposium, Solvation and Ionic Effects in Bio-molecules: Theory to Experiment, Yerevan, Armenia, May 2010 (poster)

## Skills

- Languages: Armenian (native), English (fluent), Russian (fluent)
- Scientific software: Mathematica, Matlab, LAMMPS, Gromacs, NAMDE, Amber, VMD, PyMol, ChemDraw
- Scientific libraries: Matplotlib, Biopython, MDAnalysis, MDTraj, RDKit, GNU GSL, NLopt, BLAST, Boost, PLUMED
- Programing: C\C++, Cuda, MPI, Python, Shell Script, LaTeX, Java, SQL, PHP, AJAX, WinApp, Visual C++, Borland C++ Builder, Visual Basic, Fox Pro, Java Mobile Edition