# Davit A. Potoyan

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#### **APPOINTMENTS**

- 2023-PRESENT Associate Professor Department of Chemistry, Iowa State University Department of Biochemistry, Biophysics, and Molecular Biology Bioinformatics and Computational Biology Program 2017-2023 Caldwell Assistant Professor
  - Department of Chemistry, Iowa State University Department of Biochemistry, Biophysics, and Molecular Biology Bioinformatics and Computational Biology Program
  - 2012-2017 **Postdoctoral Fellow** Center for Theoretical Biological Physics Rice University, Houston TX

#### EDUCATION

- 2007-2012 **PhD** in CHEMICAL PHYSICS University of Maryland, College Park MD
- 2003-2007 **BS** in CHEMISTRY Yerevan State University, Armenia

#### AWARDS

- 2022 Cottrell Scholar Collaborative award
- 2021 Cottrell Scholar award
- 2020 NIH R35 MIRA award
- 2012 Graduate award for excellence in research, University of Maryland, College Park MD
- 2011 Student Research Achievement Award, Biophysical Society, Baltimore MD

*Work at ISU (2017-present)* †-corresponding author, \*-equal contribution.

Preprints

[53] V Ramachandran, **DA Potoyan<sup>†</sup>** "Molecular Drivers of RNA Phase Separation" (2025) DOI: 10.1101/2025.01.20.633842

 [52] DP Prasanna, DA Potoyan<sup>†</sup> "Thermal Adaptation of Extremozymes: Temperature-Sensitive Contact Analysis of Serine Proteases" (2025)
 DOI: 10.1101/2025.03.03.641325

Published or Accepted

[51] D Shukla, F Morcos, **DA Potoyan<sup>†</sup>** "Mechanisms of Thermal Adaptation of Cytosolic Malate Dehydrogenase Revealed by Deep Learning and Coevolutionary Analysis" *J Chem Theor Comp* **21**, 3277 (2025)

[50] S Biswas, **DA Potoyan<sup>†</sup>** "Decoding the dynamics of biomolecular condensates: An energy landscape approach" *PLoS Comp Bio* **21** e1012826 (2025)

[49] U Patel, S Siang, **DA Potoyan**, J Roche. "Conformational landscape of the transcription factor ATF4 is dominated by disordered-mediated inter-domain coupling" *Biochemistry* (2025)

[48] D Burns, V Venditti<sup>†</sup>, **DA Potoyan**<sup>†</sup> "Illuminating protein allostery by Chemically Accurate Contact Response Analysis" J Chem Theor Comp **20**, 8711 (2024)

[47] S Biswas, **DA Potoyan<sup>†</sup>** "Molecular Drivers of Aging in Biomolecular Condensates: Desolvation, Rigidification, and Sticker Lifetimes" *Phys Rev X Life* **2**, 023011 (2024)

[46] S Yang, **DA Potoyan<sup>†</sup>** "On microscopic origins of flow activation energy in biomolecular condensates" J Phys Chem B 128, 12348 (2024)

[45] R Laghmach, M Di Piero, **DA Potoyan**<sup>†</sup>. "4D Mesoscale liquid model of nucleus resolves chromatin's radial organization" Phys Rev X Life **2**, 013006 (2024)

[44] V Ramachandran, **DA Potoyan<sup>†</sup>** "Energy landscapes of homopolymeric RNAs revealed by deep unsupervised learning" *Biophys J* **123**, 1152 (2024)

[43] W Brown, **DA** Potoyan<sup>†</sup>. "Phase separation of multicomponent peptide mixtures into dehydrated clusters with hydrophilic cores" *Biophys J* **123**, 349 (2024)

[42] V Ramachandran<sup>\*</sup>, W Brown<sup>\*</sup>, C Gayvert, **DA Potoyan**<sup>†</sup>; "Nucleoprotein phase-separation affinities revealed via atomistic simulations of short peptide and RNA fragments" *J Phys Chem Lett* **15**, 10811 (2024)

[41] V Ramachandran **DA Potoyan<sup>†</sup>** "Atomistic insights into the reentrant phase-transitions in polyuracil and polylysine mixtures" J Chem Phys **161**, 015101 (2024)

[40] D Burns, B Khatiwada, A Singh, JA Purslow, **DA Potoyan**<sup>†</sup>, V Venditti<sup>†</sup> "An  $\alpha$ -ketoglutarate conformational switch controls iron accessibility, activation and substrate selection of the human FTO protein" *Proc Natl Acad Sci* **121**, e2404457121 (2024)

[39] I Alshareedah, A Singh, S Yang, V Ramachandran, A Quinn, **DA Potoyan<sup>†</sup>**, Priya R. Banerjee<sup>†</sup>. "Determinants of Viscoelasticity and Flow Activation Energy in Biomolecular Condensates"  $Sci Adv \mathbf{10}$ , 6539 (2024)

[38] D Marijan, EA Momchilova, D Burns, R Zapf, Holger W, **DA Potoyan**, TE Audas "Protein Thermal Sensing Regulates Physiological Amyloid Aggregation" Nat Commun **15**, 1222 (2024)

[37] CL. Vizcarra, R Trainor, AR McDonald, C Richardson, **DA Potoyan**, JA Nash, B Lundgren, T Luchko, GM Hocky, JJ Foley IV, TJ Atherton, GY Stokes "An interdisciplinary effort to integrate coding into science courses" *Nature Comp Sci* (2024)

[36] JD Levengood, **DA Potoyan**, S Penumutchu, A Kumar, Y Wang, AL Hansen, S Kutluay, J Roche, Blanton S Tolbert "Thermodynamic Coupling of the tandem RRM domains of hnRNP A1 underlie its Pleiotropic RNA Binding Functions" *Sci Adv* **10**, 6580 (2024)

[35] D Burns, V Venditti<sup>†</sup>, **DA Potoyan**<sup>†</sup>. "Temperature-Sensitive Contact Modes Allosterically Gate TRPV3" *PLoS Comp Bio* **19**, e1011545 (2023)

[34] I Malhotra, **DA Potoyan<sup>†</sup>**. "Re-entrant transitions of locally stiff RNA chains in the presence of polycations leads to gelated architectures" Soft Matter **19**, 5622-5629 (2023)

[33] S Sedinkin, D Burns, D Shukla, **DA Potoyan**<sup>†</sup>, V Venditti<sup>†</sup>. "Solution structure ensembles of the open and close forms of the 130 kDa Enzyme I via AlphaFold modeling, Coarse-Grained simulations, and NMR" J. Am. Chem. Soc. **145**, 13347 (2023)

[32] A Singh, D Burns, S Sedinkin, B Van Veller, **DA Potoyan<sup>†</sup>**, V Venditti<sup>†</sup>."Protein conformational dynamics underlay selective recognition of thermophilic over mesophilic Enzyme I by a substrate analogue" *Biomolecules* **13**, 160 (2023)

[31] D Burns, A Singh, V Venditti<sup>†</sup>, **DA Potoyan**<sup>†</sup>. "Temperature Sensitive Contacts in Disordered Loops Tune Enzyme I Activity" *Proc. Natl. Acad. Sci.* **119**, e2210537119 (2022)

[30] R Laghmach, I Alshareedah, M Pham, M Raju, PR Banerjee<sup>†</sup>, **DA Potoyan**<sup>†</sup>. "RNA chain length and stoichiometry govern surface tension and stability of protein-RNA condensates" *iScience* **25**, 104105 (2022)

[29] AE Badaczweska-Dawid, V Uversky<sup>†</sup>, **DA Potoyan**<sup>†</sup>. "BIAPSS: A comprehensive physicochemical analyzer of proteins undergoing liquid-liquid phase separation" *Int. J. Mol. Sci.* **23**, 6204 (2022)

[28] R Laghmach, M Di Pierro, **DA Potoyan**<sup>†</sup>. "Liquid state perspective on dynamics of chromatin compartments" *Front. Mol. Biosci.* 8, 781981 (2022)

[27] R Laghmach, I Malhotra, **DA Potoyan**<sup>†</sup>. "Multi-scale modeling of protein-RNA condensation in and out of equilibrium" *Methods in Molecular Biology* **2563** (2022)

[26] I Alshareedah, MM Moosa, M Pham, DA Potoyan<sup>†</sup>, PR Banerjee<sup>†</sup>. "Programmable Viscoelasticity in Protein-RNA Condensates with Disordered Sticker-Spacer Polypeptides" Nat Commun. 12, 1-14 (2021)

[25] R Laghmach, M Di Pierro, **DA Potoyan<sup>†</sup>** "Interplay of chromatin phase separation and lamina interactions in nuclear organization" *Biophys J.* **120**, 5005–5017 (2021)

[24] J Mueterthies, **DA Potoyan**<sup>†</sup>. "Solvent Exposure and Ionic Condensation Drive Fuzzy Dimerization of Disordered Heterochromatin Protein Sequence" *Biomolecules* **11**, 915 (2021)

[23] T Kaur, M Raju, I Alshareedah, RB Davis, **DA Potoyan**<sup>†</sup>, PR Banerjee<sup>†</sup>. "Sequence-encoded and Composition-dependent Protein-RNA Interactions Control Multiphasic Condensate Topologies" *Nat Commun* **12**, 1-6 (2021)

[22] R Laghmach, **DA Potoyan<sup>†</sup>**. "Liquid-liquid phase separation driven compartmentalization of reactive nucleoplasm" *Phys Biol.* **18** 015001 (2020)

[21] RR Dotas, TT Nguyen, CE Stewart Jr, R Ghirlando, **DA Potoyan**<sup>†</sup>, V Venditti<sup>†</sup>. "Hybrid thermophilic/mesophilic enzymes reveal a role for conformational disorder in regulation of bacterial Enzyme I." J Mol Biol **432**, 4481 (2020)

[20] I Alshareedaha, MM Moosa, M Raju, **DA Potoyan**<sup>†</sup>, PR Banerjee<sup>†</sup>. "Phase Transition of RNA-protein Complexes into Ordered Hollow Condensates." *Proc Natl Acad Sci* **117**, 15650 (2020)

[19] R Laghmach, M Di Pierro, **DA Potoyan**<sup>†</sup>. "Mesoscale liquid model of chromatin recapitulates large-scale organization of eukaryotic cell nuclei" *Biophys J*, **118**, 2130 (2020)

[18] J Roche, **DA Potoyan<sup>†</sup>**. "Disorder mediated oligomerization of DISC1 proteins revealed by coarse-grained molecular dynamics simulations." J Phys Chem B **123**, 9567 (2019)

[17] YT Lin, PG Hufton, EJ Lee, **DA Potoyan<sup>†</sup>**. "Stochastic and dynamical view of pluripotency in mouse embryonic stem cells" *PLoS Comp Bio* **14**, 1006000 (2018)

[16] M Di Pierro<sup>\*</sup>, **DA Potoyan**<sup>\*</sup>, PG Wolynes, JN Onuchic. "Anomalous Diffusion, Spatial Coherence, and Viscoelasticity from the Energy Landscape of Human Chromosomes" *Proc. Natl. Acad. Sci.* **115**, 7753 (2018)

[15] Z Wang<sup>\*</sup>, **DA Potoyan**<sup>\*</sup>, PG Wolynes. "Stochastic Resonances in a Distributed Genetic Broadcasting System: The  $NF\kappa B/I\kappa B$  paradigm." J. Roy. Soc. Int. **15**, 20170809 (2018)

[14] Z Wang, **DA Potoyan**, PG Wolynes. "Modeling the therapeutic efficacy of  $NF\kappa B$  synthetic decoy oligodeoxynucleotides (ODNs)." *BMC Sys. Biol.* **12**, 4 (2018)

#### Graduate and Postdoctoral Work (2010-2017)

[13] **DA Potoyan**, C Bueno, W Zheng, PG Wolynes, EA Komives. "Resolving the  $NF\kappa B$  heterodimer binding paradox: Strain and frustration guide the binding of dimeric transcription factors" J. Am. Chem. Soc. **139**, 18558 (2017)

[12] DA Potoyan, PG Wolynes. "Stochastic dynamics of genetic broadcasting networks." Phys. Rev. E. 96, 052305 (2017)

[11] **DA Potoyan**, W Zheng, DU Ferreiro, PG Wolynes, EA Komives. "PEST Control of Molecular Stripping of  $NF\kappa B$  from DNA Transcription Sites." J. Phys. Chem. B **120**, 8532 (2016)

[10] **DA Potoyan**, W Zheng, EA Komives, PG Wolynes. "Molecular stripping in the  $NF\kappa B/I\kappa B/DNA$  genetic switch." Proc. Natl. Acad. Sci. **113**, 110 (2016)

[9] Z Wang<sup>\*</sup>, **DA Potoyan**<sup>\*</sup>, PG Wolynes. "Molecular stripping, targets and decoys as modulators of oscillations in the  $NF\kappa B/I\kappa B\alpha/DNA$  genetic network." J. Roy. Soc. Int. **13**, 0560 (2016)

[8] DA Potoyan<sup>†</sup>, PG Wolynes. "Dichotomous noise based models of genetic switching."
 J. Chem. Phys. 143, 195101 (2015)

[7] D Winogradoff, I Echeverria, **DA Potoyan**, GA Papoian. "The acetylation landscape of the H4 histone tail: disentangling the interplay between the specific and cumulative effects." J. Am. Chem. Soc. **137**, 6245 (2015)

[6] **DA Potoyan**, PG Wolynes. "On the dephasing of genetic oscillators." *Proc. Natl. Acad. Sci.* **111**, 2391 (2014)

[5] **DA Potoyan**, A Savelyev, GA Papoian. "Coarse graining the DNA: The beginning of a long journey." WIRES Comp. Mol. Sci. **116**, 1709 (2013)

[4] **DA Potoyan**, GA Papoian. "Regulation of the H4 tail binding and folding landscapes via Lys-16 acetylation." *Proc. Natl. Acad. Sci.* **109**, 17857 (2012)

[3] DA Potoyan, P. Zhuravlev, GA Papoian. "Computing free energy of a large-scale allosteric transition in Adenylate Kinase using all atom explicit solvent simulations."
 J. Phys. Chem. B 116, 1709 (2012)

[2] **DA Potoyan**, GA Papoian. "Energy landscape analyses of disordered histone tails reveal special organization of their conformational dynamics." J. Am. Chem. Soc. **133**, 7405 (2011)

[1] P Zhuravlev, S Wu, **DA Potoyan**, M Rubinstein, GA Papoian. "Computing free energies of protein conformations from explicit solvent simulations" *Methods.* **52**, 115121 (2010)

#### TEACHING

Spring, 2025	Chem 563; Statistical Mechanics.
Fall, $2024$	Chem 324; Introduction to Quantum Mechanics.
Spring, 2024	Chem 563; Statistical Mechanics.
Fall, $2023$	Chem 324; Introduction to Quantum Mechanics.
Fall, $2022$	Chem 167; General Chemistry.
Spring, 2022	Chem 563; Statistical Mechanics.
Fall, $2021$	Chem 167; General Chemistry.
Spring, 2021	Chem 563; Statistical Mechanics.
Fall, $2020$	Chem 167; General Chemistry.
Spring, 2020	Chem 563; Statistical Mechanics.
Fall, $2019$	Chem 324; Introduction to Quantum Mechanics.
Spring, 2019	Chem 563; Statistical Mechanics.
Spring, 2018	Chem 324; Introduction to Quantum Mechanics.
Fall, 2017	Chem 324; Introduction to Quantum Mechanics.

#### INVITED TALKS

- 2025 American Chemical Society Meeting, San Diego, CA
- 2024 Molecular and Cellular Biology, University of Massachusetts, Amherst, MA
- 2024 American Physical Society Meeting, Minneapolis, MA
- 2024 Biophysical Society Meeting, Philadelphia, PA
- 2024 Department of Biological Sciences, University of Texas, Dallas, TX
- 2023 American Chemical Society Meeting, Indianapolis, IA
- 2022 Department of Chemistry, University of California, Los Angeles, CA
- 2022 Department of Physics, Northeastern University, MA
- 2022 Department of Physics, University of Buffalo, NY
- 2022 Department of Chemistry, University of Maryland, MD
- 2022 Department of Chemistry, University of Oregon, OR
- 2022 Department of Chemistry, University of Minnesota, MN
- 2021 (virtual) NYU Chromatin Club, New York University, NY
- 2021 (virtual) Department of Physics, University of Buffalo, NY
- 2020 (virtual) Department of Chemistry, McGill University, Montreal, Canada
- 2019 Department of Chemistry, University of Illinois, Chicago
- 2019 Department of Applied Mathematics, Illinois Institute of Technology, Chicago
- 2018 Department of Chemistry, University of Nebraska, Omaha
- 2017 Center for Nonlinear Studies, Los Alamos National Lab, Los Alamos NM
- 2017 Department of Physics, University of Northern Iowa, Waterloo IA

#### Meetings Organized:

- "Multi-scale Modeling of Biomolecular Condensates," ACS Spring National Meeting, San Diego, March 26, 2025
- ESCIP workshop "Teaching scientific computing at the dawn of AI", Ames, IA, May 30-31, 2024

#### Peer Reviewing:

• Proc Natl Acad Sci, Biophys J, PLoS Comput Biol, J Phys Chem B, J Chem Phys, Nucleic Acids Res, Frontiers Biosci, iScience, Biomolecules, Phys Biol, Sci Rep

#### **Departmental Committees:**

- 2023 ISU Chemistry Graduate Admissions Committee
- 2023 ISU Strategic Planning Committee
- 2022 ISU Chemistry Department Vision Committee
- 2021 ISU Chemistry Department Survey Committee
- 2020 ISU Bioinformatics and Computational Biology (BCB) Program Admissions Committee
- 2019 ISU Chemistry Department Website Committee
- 2018 ISU Chemistry Department Planning Committee

#### CURRENT FUNDING

# Grant:NIH R35, GM138243-01Title:"Multi-scale computational investigation of functions and<br/>mechanisms of protein-RNA phase separation."Status:ActiveAward:\$1,703,640Period:09/15/2020-07/31/2025 (Renewal pending for 2025-2030)Investigators:Davit Potoyan(PI)

### PENDING FUNDING

Grant:	NIH R35, $GM138243-01R$
Title:	"Multi-scale computational investigation of functions and
	mechanisms of protein-RNA phase separation."
Award:	\$1,846,340
Period:	09/15/2025-07/31/2030
Investigators:	Davit Potoyan(PI)
Grant:	NSF, 2435848
<b>Grant:</b> <i>Title:</i>	NSF, 2435848 "ACED: Accelerating Inference of Protein Dynamics from Structural Data
Grant: Title:	NSF, 2435848 "ACED: Accelerating Inference of Protein Dynamics from Structural Data via Synergistic Use of Molecular Dynamics and AI"
<b>Grant:</b> <i>Title:</i> <i>Award:</i>	NSF, 2435848 "ACED: Accelerating Inference of Protein Dynamics from Structural Data via Synergistic Use of Molecular Dynamics and AI" \$3,000,000

## COMPLETED FUNDING

Grant:	Cottrell Scholar
Title:	"Uncovering principles of bio-molecular condensation:
	from single molecules to cellular organelles"
Status:	Active
Award:	\$100,000
Period:	07/01/2021- $09/30/2024$
Investigators:	Davit Potoyan(PI)
Grant:	Cottrell Scholar Collaborative
Title:	"Broadening and deepening the ESCIP network:
	Infusing computational science concepts into STEM courses through multidisciplinary instructor collaborative networks."
Status:	Active
Award:	\$10,000
Period:	09/01/2022-08/30/2024
Investigators:	Davit Potoyan (PI)
Grant:	NIH R01, GM132561-01
Title:	"Structure and function of DISC1 in the cAMP pathway"
Status:	Active
Award:	\$44,445
Period:	07/01/2019-10/30/2024
Investigators:	Julien Roche(PI), Underbakke Eric(Co-PI),
~	Stewart Charles(Co-PI) and Davit Potoyan(Co-PI)

### **GROUP MEMBERS**

#### Postdoctoral researchers

Subhadip Biswas 2023-Present, PhD, University of SheffieldSean Yang 2023-Present, PhD, Shanghai JiaoTong University

#### PhD students

Grace Tiffany 2025-Present, *Biophysics* Shalith Chamantha 2025-Present, *Chemistry* Tuqa Ibrahim 2025-Present, *Chemistry* Krishna Suresh 2024-Present, *Chemistry* Sunera Arambewela 2024-Present, *Chemistry* Zachary Miller 2024-Present, *Physics* Divyanshu Shukla 2023-Present, *BCB* Dulitha Prasanna 2022-Present, *Chemistry* Vysakh Ramachandran 2022-Present, *Chemistry* 

#### Alumni

William Brown 2020-2025, Chemistry PhD
Daniel Burns 2019-2024, Biophysics PhD
Rabia Laghmach 2018-2024, Postdoc
Chris Gayvert 2020-2023, Biophysics MS student
Isha Malhotra 2021-2022, Postdoc
Matthew Pham 2019-2021, Physics undergraduate
Aleksandra Badaczewska-Dawid 2020-2021, Postdoc
Jazelli Muetherties 2018-2020, MS student
Muralikrishna Raju 2019-2020, Postdoc
Daniel Pugliese Summer 2019, Chemistry undergraduate
Amar Srivastava Fall 2018, Chemical Engineering undergraduate
Fatima Almustafa Fall 2018, Chemistry undergraduate