



## Dr. Omar Valsson

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[UNT Faculty Profile](#)

[UNT Chemistry Profile](#)

Google Scholar: <https://scholar.google.nl/citations?user=hd8q6KgAAAAJ&hl=en>

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Web of Science ResearcherID: [D-2438-2010](#)

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GitHub (Personal): [valsion](#)

Updated January 22, 2026

## Professional Experience

- Assistant professor (Theoretical Chemistry), Department of Chemistry, University of North Texas, Denton, TX, USA – January 2022 to Present
- Group Leader, Theory Group (AK Kremer), Max Planck Institute for Polymer Research (MPIP), Mainz, Germany – April 2017 to December 2021
- Postdoctoral Researcher with Prof. Michele Parrinello, ETH Zurich and USI Lugano, Lugano, Switzerland – October 2012 to March 2017

## Education

- PhD degree in Physics with Prof. Claudia Filippi, University of Twente, Enschede, The Netherlands – September 2008 to September 2012  
Thesis: *Understanding visual absorption from first principles*  
([10.3990/1.9789036534116](#))
- Masters degree in Physics, University of Iceland – September 2006 to June 2008
- Bachelors degree in Physics, University of Iceland – September 2003 to June 2006

## Honors and Awards

- *PCCP 2025 Emerging Investigator*, Royal Society of Chemistry (RSC) Journal Physical Chemistry Chemical Physics – June 2025.
- *Department of Energy (DOE) Office of Science Early Career Award 2023* – August 2023 (Includes grant funded for 5 years, \$875,000 – July 2023 to June 2028).  
First researcher at UNT to be awarded the DOE SC Early Career Award.
- Prize of Gudmundur P. Bjarnason for excellent academic achievement in Physics at the Bachelors (Undergraduate) level at the University of Iceland – June 2006.

## Other Appointments

- Member of the [PLUMED Consortium](#) – 2019 to Present

## Ongoing Grants

- *The Molecular Building Block Sampling Approach for Polymorphic Free Energy Calculations*  
DOE SC Early Career Award 2023 / BES Condensed Phase and Interfacial Molecular Science (CPIMS) / DE-SC0024283 – \$875,000 – July 2023 to June 2028.  
First researcher at UNT to be awarded the DOE SC Early Career Award/Grant.

## Completed Grants

### Since starting as an Assistant Professor at UNT in January 2022

- *A Multiscale Multiphysics In-Silico Model of Photobiomodulation Therapy for Hearing Preservation*  
PIs: Omar Valsson (50%) and Fateme Esmailie (50%, UNT, Department of Biomedical Engineering). UNT College of Engineering and College of Science Collaborative Research Seed Grant – \$10,000 – July 2024 to April 2025.

### Prior to starting as an Assistant Professor at UNT in January 2022

- *Improving Performance of Multiple Walkers in Enhanced Sampling via a Birth/Death Process*  
PIs: Omar Valsson (physics, simulations) and Lisa Hartung from the Johannes Gutenberg University of Mainz (mathematics, statistics).  
Funding for one postdoc from July 2020 to June 2022 that works at the Johannes Gutenberg University of Mainz. Total amount of around 150,000 EUR (180,000 USD). Funded by the TRR 146, a collaborative research center on Multiscale Modeling.
- *Unraveling and Controlling Out of Equilibrium Self-Assembly*  
PIs: Omar Valsson (physics, simulations) and Andreas Riedinger from MPIP (chemistry, experiments).  
Funding for one PhD student from Oct 2019 to Oct. 2022. Total amount of around 110,000 EUR (130,000 USD). Funded from a central call within Max Planck Institute for Polymer Research for projects dealing with multiscale and/or non-equilibrium problems.

## Publication List

Corresponding author papers have OV's name in bold.

Graduate students supervised by OV have names in italic and are labelled:

#UNT Graduate Students; %MPIP Mainz Graduate Students;

Journal impact factors and ranking are obtained from Web of Science (WoS), Journal Citation Reports (JCR) 2024, as of September 1, 2025.

Citation numbers obtained from Web Science (WoS) and Google Scholar, as of September 1, 2025.

### Since starting as an Assistant Professor at UNT in January 2022

1. S. Chen, N. Petersen%, **O. Valsson**, M. Girard, and H. Wang  
*Understanding and Controlling the Colloidal Stability of CdSe Nanoplatelets by Solvation Force Engineering*  
 J. Am. Chem. Soc. 147, 35347-35354 (2025)  
 DOI: [10.1021/jacs.5c08392](https://doi.org/10.1021/jacs.5c08392)  
 Research article with research from MPIP with OV's former group members at MPIP and other collaborators, and OV as one of the corresponding authors.  
 Journal Impact Factor: 15.6  
 Journal Ranking: 17 out of 239 in Chemistry, Multidisciplinary.
2. S. Bhusal# and **O. Valsson**  
*Characterizing the conformational ensemble of PROTAC degraders in solutions via atomistic simulations*  
 Phys. Chem. Chem. Phys. 27, 24211-24224 (2025)  
 DOI: [10.1039/D5CP02530C](https://doi.org/10.1039/D5CP02530C)  
**Invited submission to the PCCP 2025 Emerging Investigators Themed Collection**  
 Research article with research from UNT with only UNT group members as authors and OV as corresponding author  
 Journal Impact Factor: 2.9  
 Journal Ranking: 116 out of 185 in Chemistry, Physical and 13 out of 39 in Physics, Atomic, Molecular & Chemical.  
 Total Citation: 2 (Google Scholar)
3. G. A. Tribello, M. Bonomi, G. Bussi, C. Camilloni, ..., **O. Valsson**, ... (see full author list in paper)  
*PLUMED Tutorials: a collaborative, community-driven learning ecosystem*  
 J. Chem. Phys. 162, 092501 (2025)  
 DOI: <https://doi.org/10.1063/5.0251501>  
 Part of the Michele Parrinello Festschrift  
 Peer-reviewed perspective/opinion article introducing the PLUMED Tutorials with international collaborators that OV contributed to. The PLUMED Tutorials is a living textbook that includes a wide range of tutorials and teaches students about the research done by the members of the PLUMED consortium. OV has contributed tutorials there.  
 Journal Impact Factor: 3.1  
 Journal Ranking: 104 out of 185 in Chemistry, Physical; and 10 out of 39 in Physics, Atomic, Molecular & Chemical.  
 Total Citation: 5 (WoS) / 15 (Google Scholar)

4. L. M. Ghiringhelli, C. Baldauf, ..., O. Valsson, C. Wöll, and M. Scheffler (see full author list in paper)  
*Shared Metadata for Data-Centric Materials Science*  
 Scientific Data 10, 626 (2023)  
 DOI: [10.1038/s41597-023-02501-8](https://doi.org/10.1038/s41597-023-02501-8)  
 Peer-reviewed perspective/opinion article on fair data sharing within materials science with international collaborators that OV contributed to.  
 Journal Impact Factor: 6.9  
 Journal Ranking: 15 out of 135 in Multidisciplinary Sciences.  
 Total Citation: 22 (WoS) / 34 (Google Scholar)
5. J. Rydzewski, M. Chen, and O. Valsson  
*Manifold Learning in Atomistic Simulations: A Conceptual Review*  
 Mach. Learn.: Sci. Technol. 4, 031001 (2023)  
 DOI: [10.1088/2632-2153/ace81a](https://doi.org/10.1088/2632-2153/ace81a)  
 Peer-reviewed review article with international collaborators with OV as one of the three contributing authors.  
 Journal Impact Factor: 4.6  
 Journal Ranking: 20 out of 135 In Multidisciplinary Sciences; 60 out of 204 In Computer Science, Artificial Intelligence; and 50 out of 175 In Computer Science, Interdisciplinary Applications.  
 Total Citation: 11 (WoS) / 21 (Google Scholar)
6. A. Iscen, N. Forero-Martinez, O. Valsson, and K. Kremer  
*Molecular Simulation Strategies for Understanding the Degradation Mechanisms of Acrylic Polymers*  
 Macromolecules 56, 3272-3285 (2023)  
 DOI: [10.1021/acs.macromol.2c02442](https://doi.org/10.1021/acs.macromol.2c02442)  
 Peer-reviewed research article with research from MPIP where OV was a collaborator and contributed to.  
 Journal Impact Factor: 5.2  
 Journal Ranking: 15 out of 94 in Polymer Science.  
 Total Citation: 11 (WoS) / 11 (Google Scholar)
7. B. Pampel, S. Holbach, L. Hartung, and **O. Valsson**  
*Sampling Rare Event Energy Landscapes via Birth-Death Augmented Dynamics*  
 Phys. Rev. E 107, 024141 (2023)  
 DOI: [10.1103/PhysRevE.107.024141](https://doi.org/10.1103/PhysRevE.107.024141)  
**Selected as Editor's Suggestion**  
 Peer-reviewed research article with research from MPIP with OV's group members at MPIP and other collaborators, and OV as corresponding author. OV lead the ideation and was the main supervisor of this research.  
 Journal Impact Factor: 2.4  
 Journal Ranking: 17 out of 41 in Physics, Fluids & Plasmas; and 13 out of 61 in Physics, Mathematical.  
 Total Citation: 1 (WoS) / 2 (Google Scholar)
8. J. Hénin, T. Lelièvre, M. R. Shirts, **O. Valsson**, and L. Delemotte  
*Enhanced Sampling Methods for Molecular Dynamics Simulations*  
 LiveCoMS. 4, 1583 (2022)  
 DOI: [10.33011/livecoms.4.1.1583](https://doi.org/10.33011/livecoms.4.1.1583)  
 Peer-reviewed review article with international collaborators with OV as one of the

corresponding authors; OV wrote initial drafts of Sections 6 and 7, and contributed to all other Sections.

This journal is a community-based journal not ranked by WoS JCR so no journal impact factor is available.

This review article has been well-received by the atomistic simulation community with over 339 citations according to Google Scholar.

Total Citation: 339 (Google Scholar)

9. N. Petersen<sup>§</sup>, M. Girard, A. Riedinger, and **O. Valsson**

*The Crucial Role of Solvation Forces in the Steric Stabilization of Nanoplatelets*

Nano Lett. 22, 9847-9853 (2022)

DOI: [10.1021/acs.nanolett.2c02848](https://doi.org/10.1021/acs.nanolett.2c02848)

Peer-reviewed research article with research from MPIP with OV's group members at MPIP and other collaborators, and OV as corresponding author. OV co-lead the ideation and was the main supervisor of the research of this research.

Journal Impact Factor: 9.1

Journal Ranking: 34 out of 239 in Chemistry, Multidisciplinary; 24 out of 147 in Nanoscience & Nanotechnology; 34 out of 185 in Chemistry, Physical; and 10 out of 79 in Physics, Condensed Matter

Total Citation: 11 (WoS) / 15 (Google Scholar)

10. J. Rydzewski, M. Chen, T. K. Ghosh, and O. Valsson

*Reweightd Manifold Learning of Collective Variables from Enhanced Sampling Simulations*

J. Chem. Theory Comput. 18, 7179-7192 (2022)

DOI: [10.1021/acs.jctc.2c00873](https://doi.org/10.1021/acs.jctc.2c00873)

Peer-reviewed research article with US and international collaborators with OV as one of leading authors.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 13 (WoS) / 21 (Google Scholar)

## Prior to starting as an Assistant Professor at UNT in January 2022

11. B. Pampel<sup>§</sup> and **O. Valsson**

*Improving the Efficiency of Variationally Enhanced Sampling with Wavelet-Based Bias Potentials*

J. Chem. Theory Comput. 18, 4127-4141 (2022)

DOI: [10.1021/acs.jctc.2c00197](https://doi.org/10.1021/acs.jctc.2c00197)

Peer-reviewed research article with research from MPIP with OV's group members at MPIP and OV as leading and corresponding author.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 5 (WoS) / 7 (Google Scholar)

12. A. Iscen, N. C. Forero-Martinez, O. Valsson, and K. Kremer

*Acrylic Paints: An Atomistic View of Polymer Structure and Effects of Environmental Pollutants*

J. Phys. Chem. B 125, 10854 (2021)

DOI: [10.1021/acs.jpcc.1c05188](https://doi.org/10.1021/acs.jpcc.1c05188)

Peer-reviewed research article with research from MPIP where OV was a

collaborator and contributed to research.

Journal Impact Factor: 2.9

Journal Ranking: 116 out of 185 in Chemistry, Physical.

Total Citation: 18 (WoS) / 29 (Google Scholar)

13. J. Rydzewski and **O. Valsson**

*Multiscale reweighted stochastic embedding: Deep learning of collective variables for enhanced sampling*

J. Phys. Chem. A 125, 6286 (2021)

DOI: [10.1021/acs.jpca.1c02869](https://doi.org/10.1021/acs.jpca.1c02869)

Peer-reviewed research article with international collaborators with OV co-leading ideation and research, and OV as corresponding author.

Journal Impact Factor: 2.8

Journal Ranking: 120 out of 185 in Chemistry, Physical; and 15 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 27 (WoS) / 32 (Google Scholar)

14. C. Liu, J. G. Brandenburg, O.Valsson, K. Kremer, and T. Bereau

*Free-energy landscape of polymer-crystal polymorphism*

Soft Matter 16, 9683 (2020)

DOI: [10.1039/D0SM01342K](https://doi.org/10.1039/D0SM01342K)

Peer-reviewed research article with research from MPIP where OV was a collaborator and contributed to research.

Journal Impact Factor: 2.8

Journal Ranking: 120 out of 185 in Chemistry, Physical; 38 out of 114 in Physics, Multidisciplinary, and 48 out of 94 in Polymer Science.

Total Citation: 13 (WoS) / 17 (Google Scholar)

15. A. Halder, S. Kumar, O. Valsson, and G. Reddy

*Mg<sup>2+</sup> Sensing by an RNA Fragment: Role of Mg<sup>2+</sup> Coordinated Water Molecules*

J. Chem. Theory Comput. 16, 6702 (2020)

DOI: [10.1021/acs.jctc.0c00589](https://doi.org/10.1021/acs.jctc.0c00589)

Peer-reviewed research article with international collaborators MPIP where OV was a collaborator and contributed to research.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 10 (WoS) / 14 (Google Scholar)

16. **O. Valsson** and M. Parrinello

*Variationally Enhanced Sampling*

Book chapter in "Handbook of Materials Modeling - Methods: Theory and Modeling", Second Edition (2020, Editors: W. Andreoni and S. Yip)

DOI: [10.1007/978-3-319-44677-6\\_50](https://doi.org/10.1007/978-3-319-44677-6_50)

Peer-reviewed review book chapter with OV as the lead author and one of the corresponding authors.

Book chapter, no journal information available.

Total Citation: 11 (Google Scholar)

17. O. Valsson as part of the [PLUMED Consortium](#)

*Promoting Transparency and Reproducibility in Enhanced Molecular Simulations*

Nature Methods 16, 670 (2019)

DOI: [10.1038/s41592-019-0506-8](https://doi.org/10.1038/s41592-019-0506-8)

Peer-reviewed perspective/opinion article introducing the [PLUMED Consortium](#) with international collaborators that OV contributed to. The mission of the consortium is to transform the way researchers communicate the protocols that are used in their MD simulations, in order to maximize the impact of new research and promote the highest possible standards of scientific reproducibility.

Journal Impact Factor: 32.1

Journal Ranking: 1 out of 86 in Biochemical Research Methods.

Total Citation: 800 (WoS) / 938 (Google Scholar)

18. J. Rydzewski and O. Valsson

*Finding Multiple Reaction Pathways of Ligand Unbinding*

J. Chem. Phys. 150, 221101 (2019)

DOI: [10.1063/1.5108638](#)

Peer-reviewed research article with international collaborators where OV contributed to research.

Journal Impact Factor: 3.1

Journal Ranking: 104 out of 185 in Chemistry, Physical; and 10 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 29 (WoS) / 37 (Google Scholar)

19. Y. Wong, O. Valsson, P. Tiwary, M. Parrinello, and K. Lindroff-Larsen

*Frequency Adaptive Metadynamics for the Calculation of Rare-Event Kinetics*

J. Chem. Phys. 149, 072309 (2018)

DOI: [10.1063/1.5024679](#)

Peer-reviewed research article with postdoctoral advisor and international collaborators where OV contributed to research, including code development.

Journal Impact Factor: 3.1

Journal Ranking: 104 out of 185 in Chemistry, Physical; and 10 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 24 (WoS) / 74 (Google Scholar)

20. C. Perego, O. Valsson, and M. Parrinello

*Chemical Potential Calculations in Non-Homogeneous Liquids*

Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development.

J. Chem. Phys. 149, 072305 (2018)

DOI: [10.1063/1.5024631](#)

Journal Impact Factor: 3.1

Journal Ranking: 104 out of 185 in Chemistry, Physical; and 10 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 8 (WoS) / 12 (Google Scholar)

21. F. Palazzesi, O. Valsson, and M. Parrinello

*Conformational Entropy as Collective Variable for Proteins*

J. Phys. Chem. Lett. 8, 4752 (2017)

DOI: [10.1021/acs.jpcllett.7b01770](#)

Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development.

Journal Impact Factor: 4.6

Journal Ranking: 72 out of 185 in Chemistry, Physical; 7 out of 39 in Physics, Atomic, Molecular & Chemical; 62 out of 147 in Nanoscience & Nanotechnology

Total Citation: 16 (WoS) / 22 (Google Scholar)

22. P. M. Piaggi, O. Valsson, and M. Parrinello  
*Enhancing Entropy and Enthalpy Fluctuations to Drive Crystallization in Atomistic Simulations*  
Phys. Rev. Lett. 119 015701 (2017)  
DOI: [10.1103/PhysRevLett.119.015701](https://doi.org/10.1103/PhysRevLett.119.015701)  
Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development.  
Journal Impact Factor: 9.0  
Journal Ranking: 9 out of 114 in Physics, Multidisciplinary.  
Total Citation: 94 (WoS) / 119 (Google Scholar)
23. M. Invernizzi, O. Valsson, and M. Parrinello  
*Coarse graining from variationally enhanced sampling applied to the Ginzburg-Landau model*  
Proc. Natl. Acad. Sci. USA 114 3370 (2017)  
DOI: [10.1073/pnas.1618455114](https://doi.org/10.1073/pnas.1618455114)  
Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in supervising the main author.  
Journal Impact Factor: 9.1  
Journal Ranking: 14 out of 135 in Multidisciplinary Sciences.  
Total Citation: 21 (WoS) / 35 (Google Scholar)
24. G. Piccini, J. McCarty, O. Valsson, and M. Parrinello  
*Variational Flooding Study of a  $S_N2$  Reaction*  
J. Phys. Chem. Lett. 8, 580 (2017)  
DOI: [10.1021/acs.jpcllett.6b02852](https://doi.org/10.1021/acs.jpcllett.6b02852)  
Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development.  
Journal Impact Factor: 4.6  
Journal Ranking: 72 out of 185 in Chemistry, Physical; 7 out of 39 in Physics, Atomic, Molecular & Chemical; 62 out of 147 in Nanoscience & Nanotechnology  
Total Citation: 28 (WoS) / 38 (Google Scholar)
25. R. Guareschi, O. Valsson, C. Curutchet, B. Mennucci, and C. Filippi  
*Electrostatic versus Resonance Interactions in Photoreceptor Proteins: the Case of Rhodopsin*  
J. Phys. Chem. Lett. 7, 4547 (2016)  
DOI: [10.1021/acs.jpcllett.6b02043](https://doi.org/10.1021/acs.jpcllett.6b02043)  
Peer-reviewed research article with PhD advisor and collaborators where OV contributed to research.  
Journal Impact Factor: 4.6  
Journal Ranking: 72 out of 185 in Chemistry, Physical; 7 out of 39 in Physics, Atomic, Molecular & Chemical; 62 out of 147 in Nanoscience & Nanotechnology  
Total Citation: 26 (WoS) / 35 (Google Scholar)
26. P. Shaffer, O. Valsson, and M. Parrinello  
*Hierarchical Protein Free Energy Landscapes from Variationally Enhanced Sampling*  
J. Chem. Theory Comput. 12, 5751 (2016)  
DOI: [10.1021/acs.jctc.6b00786](https://doi.org/10.1021/acs.jctc.6b00786)  
Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in



supervising the main author.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 4 (WoS) / 7 (Google Scholar)

27. P. M. Piaggi, O. Valsson, and M. Parrinello

*A Variational Approach to Nucleation Simulation*

Farad. Discuss. 195, 557 (2016)

DOI: [10.1039/C6FD00127K](https://doi.org/10.1039/C6FD00127K)

Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in supervising the main author.

Journal Impact Factor: 3.1

Journal Ranking: 104 out of 185 in Chemistry, Physical.

Total Citation: 13 (WoS) / 21 (Google Scholar)

28. J. McCarty, O. Valsson, and M. Parrinello

*Bespoke Bias for Obtaining Free Energy Differences within Variationally Enhanced Sampling*

J. Chem. Theory Comput. 12 2162 (2016)

DOI: [10.1021/acs.jctc.6b00125](https://doi.org/10.1021/acs.jctc.6b00125)

Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in supervising the main author.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 11 (WoS) / 20 (Google Scholar)

29. O. Valsson, P. Tiwary, and M. Parrinello

*Enhancing Important Fluctuations: Rare Events and Metadynamics from a Conceptual Viewpoint*

Annu. Rev. Phys. Chem. 67 159 (2016)

Peer-reviewed research article with postdoctoral advisor and collaborators where OV lead the writing process.

Journal Impact Factor: 11.7

Journal Ranking: 26 out of 185 in Chemistry, Physical.

DOI: [10.1146/annurev-physchem-040215-112229](https://doi.org/10.1146/annurev-physchem-040215-112229)

Total Citation: 499 (WoS) / 681 (Google Scholar)

30. P. Shaffer, O. Valsson, and M. Parrinello

*Enhanced, targeted sampling of high-dimensional free-energy landscapes using variationally enhanced sampling, with an application to chignolin*

Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in supervising the main author.

Proc. Natl. Acad. Sci. USA 113 1150 (2016)

DOI: [10.1073/pnas.1519712113](https://doi.org/10.1073/pnas.1519712113)

Journal Impact Factor: 9.1

Journal Ranking: 14 out of 135 in Multidisciplinary Sciences.

Total Citation: 49 (WoS) / 67 (Google Scholar)

31. J. McCarty, O. Valsson, P. Tiwary, and M. Parrinello  
*Variationally Optimized Free-Energy Flooding for Rate Calculation*  
Phys. Rev. Lett. 115 070601 (2015)  
DOI: [10.1103/PhysRevLett.115.070601](https://doi.org/10.1103/PhysRevLett.115.070601)  
Peer-reviewed research article with postdoctoral advisor and collaborators where OV contributed to research, including code development and took part in supervising the main author.  
Journal Impact Factor: 9.0  
Journal Ranking: 9 out of 114 in Physics, Multidisciplinary.  
Total Citation: 38 (WoS) / 48 (Google Scholar)
32. **O. Valsson** and M. Parrinello  
*Well-Tempered Variational Approach to Enhanced Sampling*  
J. Chem. Theory Comput. 11 1996 (2015)  
DOI: [10.1021/acs.jctc.5b00076](https://doi.org/10.1021/acs.jctc.5b00076)  
Peer-reviewed research article with postdoctoral advisor where OV was the lead researcher and author.  
Journal Impact Factor: 5.5  
Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.  
Total Citation: 42 (WoS) / 51 (Google Scholar)
33. O. Valsson, C. Filippi, and M. E. Casita  
*Regarding the use and misuse of retinal protonated Schiff base photochemistry as a test case for time-dependent density-functional theory*  
J. Chem. Phys. 142 144104 (2015)  
DOI: [10.1063/1.4916354](https://doi.org/10.1063/1.4916354)  
Peer-reviewed research article with PhD advisor where OV was the lead researcher and author.  
Journal Impact Factor: 3.1  
Journal Ranking: 104 out of 185 in Chemistry, Physical; and 10 out of 39 in Physics, Atomic, Molecular & Chemical.  
Total Citation: 17 (WoS) / 24 (Google Scholar)
34. **O. Valsson** and M. Parrinello  
*Variational Approach to Enhanced Sampling and Free Energy Calculations*  
Phys. Rev. Lett. 113 090601 (2014)  
DOI: [10.1103/PhysRevLett.113.090601](https://doi.org/10.1103/PhysRevLett.113.090601)  
Peer-reviewed research article with postdoctoral advisor where OV was the lead researcher and author.  
Journal Impact Factor: 9.0  
Journal Ranking: 9 out of 114 in Physics, Multidisciplinary.  
Total Citation: 242 (WoS) / 311 (Google Scholar)
35. **O. Valsson** and M. Parrinello  
*Thermodynamical Description of a Quasi-First-Order Phase Transition from the Well-Tempered Ensemble*  
J. Chem. Theory Comput. 9 5267 (2013)  
DOI: [10.1021/ct400859f](https://doi.org/10.1021/ct400859f)  
Peer-reviewed research article with postdoctoral advisor where OV was the lead researcher and author.  
Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 13 (WoS) / 18 (Google Scholar)

36. C. Daday, C. König, O. Valsson, J. Neugebauer, and C. Filippi  
*State-Specific Embedding Potentials for Excitation-Energy Calculations*  
J. Chem. Theory Comput. 9 2355 (2013)  
DOI: [10.1021/ct400086a](https://doi.org/10.1021/ct400086a)  
Peer-reviewed research article with PhD advisor and collaborators where OV contributed to research.  
Journal Impact Factor: 5.5  
Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.  
Total Citation: 74 (WoS) / 93 (Google Scholar)
37. O. Valsson, P. Campomanes, I. Tavernelli, U. Röthlisberger, and C. Filippi  
*Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls*  
J. Chem. Theory Comput. 9 2441 (2013)  
DOI: [10.1021/ct3010408](https://doi.org/10.1021/ct3010408)  
Peer-reviewed research article with PhD advisor where OV was the lead researcher and author.  
Journal Impact Factor: 5.5  
Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.  
Total Citation: 78 (WoS) / 110 (Google Scholar)
38. O. Valsson, C. Angeli, and C. Filippi  
*Excitation energies of retinal chromophores: critical role of the structural model*  
Phys. Chem. Chem. Phys. 14 11015 (2012)  
DOI: [10.1039/C2CP41387F](https://doi.org/10.1039/C2CP41387F)  
Peer-reviewed research article with PhD advisor where OV was the lead researcher and author.  
Journal Impact Factor: 2.9  
Journal Ranking: 116 out of 185 in Chemistry, Physical and 13 out of 39 in Physics, Atomic, Molecular & Chemical.  
Total Citation: 47 (WoS) / 57 (Google Scholar)
39. O. Valsson and C. Filippi  
*Gas-Phase Retinal Spectroscopy: Temperature Effects Are But a Mirage*  
J. Phys. Chem. Lett. 3, 908 (2012)  
DOI: [10.1021/jz300183g](https://doi.org/10.1021/jz300183g)  
Peer-reviewed research article with PhD advisor where OV was the lead researcher and author.  
Journal Impact Factor: 4.6  
Journal Ranking: 72 out of 185 in Chemistry, Physical; 7 out of 39 in Physics, Atomic, Molecular & Chemical; 62 out of 147 in Nanoscience & Nanotechnology  
Total Citation: 19 (WoS) / 22 (Google Scholar)
40. R. Send, **O. Valsson**, and C. Filippi  
*Electronic Excitations of Simple Cyanine Dyes: Reconciling Density Functional and Wave Function Methods*  
J. Chem. Theory Comput. 7, 444 (2011)  
DOI: [10.1021/ct1006295](https://doi.org/10.1021/ct1006295)

Peer-reviewed research article with PhD advisor and collaborators where OV co-lead the research.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 125 (WoS) / 155 (Google Scholar)

41. **O. Valsson** and C. Filippi

*Photoisomerization of Model Retinal Chromophores: Insight From Quantum Monte Carlo and Multiconfigurational Perturbation Theory*

J. Chem. Theory Comput. 6, 1275 (2010)

DOI: [10.1021/ct900692y](https://doi.org/10.1021/ct900692y)

Peer-reviewed research article with PhD advisor where OV was the lead researcher and author.

Journal Impact Factor: 5.5

Journal Ranking: 59 out of 185 in Chemistry, Physical; and 5 out of 39 in Physics, Atomic, Molecular & Chemical.

Total Citation: 122 (WoS) / 156 (Google Scholar)

42. **O. Valsson**, C.-S. Tang, and V. Gudmundsson

*Coherent switching by detuning a side-coupled quantum-dot system*

Phys. Rev. B 78, 165318 (2008)

DOI: [10.1103/PhysRevB.78.165318](https://doi.org/10.1103/PhysRevB.78.165318)

Peer-reviewed research article with MSc advisor where OV was the lead researcher and author.

Journal Impact Factor: 3.7

Journal Ranking: 14 out of 67 in Physics, Condensed Matter.

Total Citation: 11 (WoS) / 14 (Google Scholar)

## Mentoring Activities

Graduate Students at the University of North Texas – Graduated – 1

1. Pradip Si – September 2022 to December 2025. Graduated from UNT Chemistry in December 2025 – Currently a postdoctoral researcher at UT Austin.

Graduate Students at the University of North Texas – Current – 8

1. Shikshya Bhusal – August 2021 to Present
2. Aloka Senanayaka – January 2023 to Present
3. Jaya Pathak – January 2023 to Present
4. Dipesh Shrestha – January 2023 to Present
5. Logan Estridge – September 2023 to Present
6. Oriana Silva – January 2024 to Present
7. Sara Alinejad – September 2024 to Present
8. Kabita Sharma – September 2024 to Present

Undergraduate Students at the University of North Texas doing Research in the Valsson Research Group – 12

1. Austin Thompson – April 2024 to May 2025
2. Keiran Nelson, Computer Science – April 2024 to Present

3. Danielle Walder, Chemistry – April 2024 to Present
4. Sachin Gordhan, Chemistry— September 2024 to May 2025
5. Devin Williams, Chemistry – September 2024 to May 2025
6. Ryan Lee, Texas Academy of Mathematics and Science (TAMS) – September 2024 to Present
7. Bea Venice Jane Buhawe, Biochemistry – March 2025 to Present
8. Daianna Vazquez, Chemistry – March 2025 to July 2025
9. Suhita Sainathuni, Texas Academy of Mathematics and Science (TAMS) – April 2025 to Present
10. Mmesoma Atani, Pre-Medical – September 2025 to Present
11. Viraj Shrivastava, Texas Academy of Mathematics and Science (TAMS) – September 2025 to Present
12. Jacquilyn Ly, Biochemistry – November 2025 to Present

#### Visitors at University of North Texas – 2

1. Lara Alswafta, Undergraduate Student from the Southwestern University, Texas. Visited the Valsson Research Group in the Summer of 2025 under the UNT Chemistry NSF Research Experiences for Undergraduates (REU) Program, Chemistry Research Experiences for Early-Stage Undergraduates through Collaborative HSI Partnerships (NSF Grant CHE-2447861).
2. Grace Sheridan, Undergraduate Student from the Rose-Hulman Institute of Technology, Indiana. Visited the Valsson Research Group in the Summer of 2023 under the UNT Chemistry NSF Research Experiences for Undergraduates (REU) Program, Team-Mentored Interdisciplinary Research Experiences in Chemistry for Early-Stage Undergraduates (NSF Grant CHE-1757946).

#### Alumni Prior to University of North Texas – 4

1. Nanning Petersen, PhD Student at the MPI for Polymer Research from October 2019 to April 2024. Graduated in April 2024.
2. Benjamin Pampel, PhD Student at the MPI for Polymer Research from March 2018 to June 2022. Graduated in June 2022. Postdoctoral Researcher at MPI for Polymer Research from July 2022 to October 2022.
3. Bin Song, PhD Student the MPI for Polymer Research from October 2017 to May 2022. Graduated in May 2022.
4. Nehzat Safaei, Postdoctoral Researcher at the MPI for Polymer Research from February 2018 to June 2021

#### Selected Student Accomplishments

- Shikshya Bhusal – *Promise in COMP / Women Make COMP Award* of the American Chemical Society (ACS) Division of Computers in Chemistry (COMP), ACS Spring Meeting 2025 – March 2025
- Oriana Silva – Travel scholarship to attend the SACNAS 2024 NDiSTEM Conference in Phoenix, Arizona, October 31 to November 2, 2024
- Oriana Silva – Travel scholarship to attend the International HPC Summer School 2024 in Kobe, Japan, July 7-12, 2024

## Invited Presentations at Conferences, Workshop, Seminars, and Schools

Only invited seminars and presentations listed

### Since starting as an Assistant Professor at UNT in January 2022

- 1. Chemistry Seminar at Western Washington University**  
Invited seminar within the Department of Chemistry  
Western Washington University, Bellingham, WA, USA. December 2025  
Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*
- 2. Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology**  
Invited presentation at a conference  
Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy.  
September 2025  
Title: *From Stability to Dissociation: Elucidating Unbinding Kinetics of Protein-Protein Complexes via Atomistic Simulations*
- 3. Physical Chemistry Seminar at University of Oregon**  
Invited seminar within the Department of Chemistry and Biochemistry  
University of Oregon, Eugene, OR, USA. April 2025  
Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*
- 4. American Chemical Society (ACS) Spring Meeting 2025**  
Invited presentation at the symposium "Reaction Coordinate and Advanced Sampling: Biophysical Understanding and Drug Discovery" organized by ACS Division of Computers in Chemistry (COMP)  
San Diego, CA, USA. March 2025  
Title: *Collective Variables for Targeted Protein Degradation: From PROTAC Conformational Ensemble in Solution to the Ternary Complex*
- 5. American Chemical Society (ACS) Spring Meeting 2025**  
Invited presentation at the symposium "Inferring Kinetics, Thermodynamics, and Mechanisms from Enhanced Sampling Simulations" organized by ACS Division of Physical Chemistry (PHYS)  
San Diego, CA, USA. March 2025  
Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*
- 6. Mesilla Chemistry Workshop 2025: Machine Learning in Molecular and Multiscale Dynamics**  
Invited seminar at a workshop  
Mesilla, NM, USA. March 2025  
Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations and Machine Learning Methods*
- 7. Society for Industrial and Applied Mathematics (SIAM) Conference on Computational Science and Engineering 2025 (CSE25)**  
Invited presentation at the symposium "Mathematics in Structural Biology (MS103)"  
Fort Worth, TX, USA. March 2025

Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*

**8. Texas Computational Chemistry Symposium**

Invited seminar at a conference

Texas Women's University, Denton, TX, USA. February 2025

Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*

**9. Physical Chemistry Seminar at Purdue University**

Invited seminar within the Department of Chemistry

Purdue University, West Lafayette, IN, USA. January 2025

Title: *From Stability to Dissociation: Elucidating Dissociation Kinetics of Protein-Protein Complexes via Atomistic Simulations*

**10. Workshop on phase space sampling using molecular simulation: Celebrating the 40th year of the Nosé dynamics (NOSE 40)**

Invited seminar at a workshop

Keio University (Hiyoshi Campus), Yokohama, Japan. November 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**11. CD-FMat Seminar at National Institute of Advanced Industrial Science and Technology (AIST, Japan)**

Invited departmental seminar at CD-FMat (Research Center for Computational Design of Advanced Functional Materials)

National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan. November 2024

Title: *Characterizing Local Molecular Environments in Molecular Crystals: From Chemical Intuition to Graph Neural Networks*

**12. American Chemical Society Southwest Regional Meeting (ACS SWRM) 2024**

Invited presentation at the symposium "Computational and Theoretical Chemistry" Waco, TX, USA. October 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**13. Biomolecular Sciences (BMOL) Seminar at Boise State University**

Invited presentation at the Biomolecular Sciences (BMOL) Graduate Program

Boise State University, Boise, ID, USA. October 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**14. American Chemical Society (ACS) Fall Meeting 2024**

Invited presentation at the symposium "Enhanced Sampling Methods for the Study of Chemical Reactions & Conformational Transitions" organized by ACS Division of Physical Chemistry (PHYS)

Denver, CO, USA. August 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**15. Department of Chemistry Seminar at University of Iceland**

Invited seminar within the Department of Chemistry

University of Iceland, Reykjavik, Iceland. May 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**16. UNT BioDiscovery Institute Seminar Series**

Invited institute seminar at the UNT BioDiscovery Institute

University of North Texas, Denton, TX, USA. March 2024

Title: *Unraveling Protein-Protein Dissociation Kinetics via Atomistic Simulations*

**17. 6th i-CoMSE Workshop: Methods for Advanced Sampling**

Invited lecture and tutorial at a i-CoMSE school

Online via Zoom. February 2024

Title: *Metadynamics*

**18. 2023 Condensed Phase and Interfacial Molecular Science (CPIMS) Principal Investigators' Research Meeting**

Invited presentation at the yearly PI meeting of DOE SC CPIMS

Rockville, MD, USA. November 2023

Title: *The Molecular Building Block Sampling Approach for Polymorphic Free Energy Calculations*

**19. Deep Modeling for Molecular Simulation 2023**

Invited lecture at a school organized by Chemistry in Solution and at Interfaces

Princeton University, Princeton, NJ. July 2023

Title: *Enhanced Sampling Methods for Molecular Dynamics Simulations*

**20. 3rd i-CoMSE Workshop: Methods for Advanced Sampling**

Invited lecture and tutorial at a i-CoMSE school

Online via Zoom. March 2023

Title: *Metadynamics*

**21. Machine Learning and Chemistry: Are We There Yet?**

Invited presentation at a MolSSI workshop

University of Maryland, College Park, MD, USA. May 2023

Title: *Manifold Learning of Collective Variables for Enhanced Sampling Simulations*

**22. Rare Events: Analysis, Numerics, and Applications**

Invited presentation at a workshop at the Brin Mathematics Research Center

University of Maryland, College Park, MD, USA. March 2023

Title: *Sampling Rare Event Energy Landscapes via a Birth-Death Process Augmented Langevin Dynamics*

**23. Erice School on Exploring and Quantifying Rough Free Energy Landscapes**

Invited presentation at a workshop

Erice, Sicily, Italy. September 2022

Title: *Sampling Rare Event Energy Landscapes via a Birth-Death Process Augmented Langevin Dynamics*

**24. PLUMED Masterclass (22-11)**

Invited lecture and tutorial at the PLUMED Masterclass school

Online via Zoom. July 2022

Title: *Variationally Enhanced Sampling*

**Prior to starting as an Assistant Professor at UNT in January 2022**

**25. Recent Advances in Modelling Rare Events (RARE2021)**

Invited presentation at a workshop

Online via Zoom. December 2021

Title: *Wavelet-Based Bias Potentials and Multiscale reweighted stochastic embedding*



**26. Bunsen-Tagung 2021 - Multi-Scale Modelling**

Invited presentation at a conference

Online via Zoom. May 2021

Title: *Multiscale reweighted stochastic embedding: Deep learning of collective variables for enhanced sampling*

**27. Soft Matter Seminar at University of Amsterdam**

Invited departmental seminar

Online via Zoom. March 2021

Title: *Understanding Long Timescale Phenomena in Chemical and Soft Matter Systems with Variationally Enhanced Sampling*

**28. Open Source Software For Enhanced-Sampling Simulations**

Invited presentation at a workshop

Lugano, Switzerland. July 2019

Title: *Recent Developments and Applications of Variationally Enhanced Sampling*

**29. CPMD Meeting 2019**

Invited presentation at a conference

Lausanne, Switzerland. July 2019

Title: *Variationally Enhanced Sampling: Recent Developments and Applications*

**30. American Chemical Society (ACS) Spring Meeting 2019**

Invited presentation at the symposium "Sampling conformations and pathways in biomolecular systems" organized by ACS Division of Physical Chemistry (PHYS)  
Orlando, FL, USA. March 2019

Title: *Variationally Enhanced Sampling: Recent Developments and Applications*

**31. The 9th International Conference on Multiscale Materials Modeling – Symposium: Towards Experimentally Relevant Time Scales: Methods for Extending Atomistic Simulation Times and Their Applications in Material Science**

Invited presentation at a conference

Osaka, Japan. October 2018

Title: *Bridging Time Scales with Variationally Enhanced Sampling*

**32. Erice School on Exploring and Quantifying Rough Free Energy Landscapes**

Invited presentation at a workshop

Erice, Sicily, Italy. May 2018

Title: *Bridging Time Scales with Variationally Enhanced Sampling*

**33. Recent Advances in Rare Events 2017**

Invited talk at a workshop

Agra, India. December 2017

Title: *Bridging Time Scales with Variationally Enhanced Sampling*

**34. Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA**

Invited lecture at a school

University of Stuttgart, Germany. October 2017

Title: *Enhanced Sampling Methods for Soft Matter Simulations*

**35. PLUMED User Meeting**

Invited presentation at a school

SISSA, Trieste, Italy. May 2017

Title: *VES Code: Module for Performing Variationally Enhanced Sampling Simulations within PLUMED*

**36. Scaling Cascades in Complex System 2017**

Invited presentation at a conference

Free University of Berlin, Berlin, Germany. March 2017

Title: *Enhancing Important Fluctuations and Exploring Free-Energy Landscapes with Variationally Enhanced Sampling*

**37. Erice School on Exploring and Quantifying Rough Free Energy Landscapes**

Invited presentation at a workshop

Erice, Sicily, Italy. October 2016

Title: *Exploring Free Energy Landscapes with Variationally Enhanced Sampling*

**38. NCCR MARVEL Annual Review and Retreat**

Invited presentation at a workshop

EPFL, Lausanne, Switzerland. September 2016

Title: *Variationally Enhanced Sampling*

**39. PASC meeting on Biological Applications of Metadynamics**

Invited presentation at a workshop

Castastegna, Switzerland. September 2014

Title: *Variational Approach to Enhanced Sampling and Free Energy Calculations*

**40. CECAM workshop on Enhancing molecular simulations with PLUMED**

Invited presentation at a workshop

Belfast, Northern Ireland. May 2014

Title: *Thermodynamical Description from the Well-Tempered Ensemble*

## Symposium/Workshop/Tutorial Organization

### Since starting as an Assistant Professor in January 2022

- Lead co-organizer of the ACS COMP (Division of Computers in Chemistry) Symposium "*Machine Learning in Chemistry*" at the ACS Spring Meeting 2026 to be held in Atlanta, March 22-26, 2026.
- Lead co-organizer of the ACS PHYS (Division of Physical Chemistry) Symposium "*Rare Event Sampling in Material Science Problems: From Fundamental Understanding to Technological Applications*" at the ACS Fall Meeting 2025 held in Washington DC, August 17-21, 2025.
- Co-organizer of the ACS COMP (Division of Computers in Chemistry) Symposium "*Machine Learning in Chemistry*" at the ACS Fall Meeting 2025 held in Washington DC, August 17-21, 2025.
- Co-organizer of the ACS COMP (Division of Computers in Chemistry) Symposium "*Machine Learning in Chemistry*" at the ACS Spring Meeting 2025 held in San Diego, March 23-27, 2025.
- Co-organizer of the ACS COMP (Division of Computers in Chemistry) Symposium "*Machine Learning in Chemistry*" at the ACS Fall Meeting 2024 held in Denver, August 18-22, 2024.
- Sole organizer of the Focus Session "*Advances in AI/ML-Driven Sampling for Atomistic Simulations*" at the APS March Meeting 2024 held in Minneapolis, March 3-8, 2024.

- Co-organizer of the Symposium "*Advances in Methods for Bridging Spatiotemporal Scales in Soft Matter, Polymer and Network Materials*" at "The 10th International Conference on Multiscale Materials Modeling" held in Baltimore, October 2-7, 2022.

### **Prior to starting as an Assistant Professor at UNT in January 2022**

- Lead organizer of the workshop "*Mainz Materials Simulation Days 2019: Exploring Complex Free Energy Landscapes: Structure/Function Formation, Multiscales, and Long Timescales*" held in Mainz, Germany, June 5-7, 2019.
- Lead organizer of the tutorial school "*MARVEL School on Variationally Enhanced Sampling 2017*" in February 2017 in Lugano, Switzerland. This was a four-day tutorial teaching people to use the enhanced sampling methods available in PLUMED 2 and the VES code.

### **Service to the Scientific Community**

- Referee for Scientific Journals:  
The Journal of Chemical Physics, Nature Communications, Journal of Chemical Information and Modeling, Journal of the American Chemical Society, Machine Learning: Science and Technology, Chemical Science, Journal of Chemical Theory and Computation, Journal of Physical Chemistry A/B/C, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, RSC Advances, Scientific Reports, Nano Letters, Nature Computational Science, Macromolecular Rapid Communications, Current Opinion in Structural Biology, Digital Discovery, Small, Proceedings of the National Academy of Sciences of the United States of America, Physical Review Letters, eLife, Chemical Reviews, Biophysical Journal, ACS Sensors, and others.  
Have reviewed about 80 journal articles since joining UNT in January 2022.
- Reviewer for grant proposals:  
US Department of Energy (DOE), National Science Foundation (NSF), American Chemical Society Petroleum Research Fund (ACS PRF), Dutch Research Council (NWO), Natural Sciences and Engineering Research Council of Canada (NSERC), and others  
Have reviewed about 14 grant proposals since joining UNT in January 2022.
- Member of the PLUMED Consortium (<https://www.plumed-nest.org/consortium.html>) – 2019 to Present

### **Service at the University of North Texas**

- Working Group for Workload and Faculty Annual Review Reform, Department of Chemistry, UNT – Member, February 2025 to Present
- Computational Biochemistry Assistant Professor Faculty Search Committee, Department of Biological Sciences, UNT – Member, September 2024 to May 2025
- Undergraduate Affairs Committee, Department of Chemistry, UNT – Member, October 2023 to Present
- Chemical Biology Assistant Professor Faculty Search Committee, Department of Chemistry, UNT – Member, September 2023 to May 2024

- Administrator Evaluation Committee, Department of Chemistry, UNT – Chair, April 2022 to March 2023
- Computational Chemistry Assistant Professor Faculty Search Committee, Department of Chemistry, UNT – Member, September 2022 to May 2023
- Digital Public Relations Committee, Department of Chemistry, UNT – Member, April 2022 to Present
- Departmental Photographer, Department of Chemistry, UNT – January 2022 to Present
- Member of around 20 graduate committees within Department of Chemistry, UNT, for students outside my research group.

## Teaching Experience

### Since starting as an Assistant Professor at UNT in January 2022

- Sole instructor for CHEM 4930/5610, Special Topics course on "*Chemical Applications of Machine Learning*" – Joint undergraduate and graduate course, 3 credit hours – Spring 2026 (12 students)
- Sole instructor for CHEM 5210 "*Advanced Physical Chemistry*" – Graduate course, 3 credit hours – Spring 2025 (15 students)
- Sole instructor for CHEM 4660/5660, "*Computational Chemistry and Biochemistry*" – Joint undergraduate and graduate course, 3 credit hours – Fall 2023 (15 students), Fall 2024 (23 students), Fall 2025 (25 students)
- Sole instructor for CHEM 3520, "*Physical Chemistry II*" (Quantum Mechanics and Spectroscopy) – Undergraduate course, 3 credit hours – Spring 2022 (30 students), Spring 2023 (36 students), and Spring 2024 (40 students)
- Organized a Python Bootcamp offered to Chemistry REU and Graduate students in the Summer 2025, 2\*2.5 hours, Attended by around 28 students. This Bootcamp will be extended in scope and offered to Chemistry Undergraduate students in the future.
- Developing a new 3 credit hours course on "*Chemical Applications of Machine Learning*" for undergraduate and graduate students that will start in Spring 2026.

### Prior to starting as an Assistant Professor at UNT in January 2022

- Joint instructor for "*Modern Computational Techniques in Condensed/Soft Matter Physics*" at Johannes Gutenberg University of Mainz – Undergraduate and graduate course – I taught 1/3 of the course – Spring 2019 and Spring 2020
- Sole instructor for "*Molecular Dynamics and Monte Carlo Methods*" at USI Lugano – Undergraduate and graduate course – Fall 2015

## Publicity, Media Appearances, and Interviews

- Newspaper Article, "Chemistry professor receives Early Career Award and grant money for research in molecular crystals", NT Daily, September 2023.

## Professional Development Activities

- University of North Texas Washington DC Fellows Program, Fall 2023 and Spring 2024.
- National Science Foundation Chemistry Early Career Investigator Workshop, NSF Division of Chemistry. Alexandria, VA, May 2023