Sabari Kumar

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Education

† *Indicates expected*

2021–2026 †	Ph.D., Physical Chemistry, Colorado State University
	Supervisor: Dr. Seonah Kim
2017–2019	B.A., Chemistry and Mathematics, University of Colorado Boulder
2013–2016	B.A., Chemistry and Mathematics, Pomona College

Appointments

2022–Curr.	Research Assistant, Dr. Seonah Kim, Colorado State University
Summer 2024	Research Intern, GlaxoSmithKline, Philadelphia, PA
2021–2022	Teaching Assistant, Dept. of Chemistry, Colorado State University
2015–2016	Undergraduate Research Assistant, Dr. Roberto Garza-Lopez, Pomona College
2014–2015	Undergraduate Teaching Assistant, Pomona College

Teaching

2022	CHEM112, General Chemistry 1 Lab	Colorado State University
2021	CHEM114, General Chemistry 2 Lab	Colorado State University
2014	CHEM001A, General Chemistry with Lab 1	Pomona College
2015	CHEM001B, General Chemistry with Lab 2	Pomona College

Supervision

2022	Olivia Harman, Summer REU Student	Colorado State University
2025	Andrew Weiland, Summer REU Student	Colorado State University

Selected Honours and Awards

2026	Travel Fellowship, Quantum Winter School 2026: Quantum Simulation, Institute for Pure and Applied Mathematics, UCLA
2024-2025	C. Michael Elliott Fellowship, Colorado State University
2024-2025	Graduate Student Outreach Award, Colorado State University
2023-2024	Sustainability Leadership Fellow, Colorado State University School of Global Environmental Sustainability
2023	Travel Fellowship, Workshop on Learning and Emergence in Molecular Systems, Institute for Pure and Applied Mathematics, UCLA
2022	Graduate Teaching Assistant Award, Department of Chemistry, Colorado State University
2021-2023	Gary E. Maciel Fund Fellowship, Colorado State University
2019	American Chemical Society Award for Undergraduate Excellence in Analytical Chemistry

Publications

Preprint URLs available at https://orcid.org/0000-0002-4965-4836

Journals

[1] PECAN: Peptide Electrostatics with Conformationally Agnostic Networks, **Sabari Kumar**, Sumin Song, Seonah Kim (In preparation)

[2] Fine-tuning Chemical Foundation Models for Property Prediction with ClAY: Cluster Augmentation for Y-properties, Hojin Jung, **Sabari Kumar**, Sumin Song, Seonah Kim (In preparation)

[3] ALFABET3: Extending Predictions of Homolytic Bond Dissociation Energy to Ring Systems, **Sabari Kumar**, Shree Sowndarya Santhanalakkshmi Vejaykummar, Peter St. John, Yeonjoon Kim, Robert S. Paton, Seonah Kim (In preparation)

[4] Combining Geometry and Topology for Accurate Protein Solubility Prediction, **Sabari Kumar**, Olivia Harman, Sumin Song, Yeonjoon Kim, Robert Paton, Seonah Kim, ChemRxiv, 2025 (Submitted), https://doi.org/10.26434/chemrxiv-2025-jmzwn

[5] A Fragment Based Approach Towards Curating, Comparing and Developing Machine Learning Models Applied in Photo-chemistry, Raúl Pérez-Soto*, Mihai V. Popescu*, **Sabari Kumar***, Leticia Adao Gomes, Changyeob Lee, Steven A. Lopez, Robert S. Paton, Seonah Kim, (Stars indicate equal contribution), Chem. Sci., 2025, DOI: 10.1039/D5SC05615B

[6] Enhancing Predictive Models for Solubility in Multi-Solvent Systems using Semi-Supervised Graph Neural Networks, Hojin Jung, Christopher D. Stubbs, **Sabari Kumar**, Raúl Pérez-Soto, Su-min Song, Yeonjoon Kim, and Seonah Kim, Digital Discovery, 2025

[7] Sooting Tendencies: Combustion Science for Designing Sustainable Fuels with Improved Properties, Lisa D. Pfefferle, Seonah Kim, **Sabari Kumar**, Charles S. McEnally, Raul Perez-Soto, Zhanhong Xiang, Yuan Xuan, Proc. Comb. Inst., 40, 1-4, 105750, 2024

[8] Designing Solvent Systems Using Self-Evolving Solubility Databases and Graph Neural Networks, Yeonjoon Kim, Hojin Jung, **Sabari Kumar**, Robert S. Paton, Seonah Kim, Chem. Sci., 15, 923-939, 2024; ChemSci Pick of the Week

[9] Sooting Tendency of Substituted Aromatic Oxygenates: The Role of Functional Groups and Positional Isomerism in Vanillin Isomers, Hojin Jung, Jaeyoung Cho, Yeonjoon Kim, Zhanhong Xiang, **Sabari Kumar**, Piper Barnard, Charles S. McEnally, Lisa D. Pfefferle, Seonah Kim, Proc. Comb. Inst., 40, 1-4, 105669, 2024

[10] Experimental and Numerical Study of the Decomposition, Product Spectrum, and Sooting Properties of Adamantane Fuels, Ga-Un Jeong, Zhanhong Xiang, **Sabari Kumar**, Collin Hansen, Adri van Duin, Seonah Kim, Charles S. McEnally, Lisa D. Pfefferle, Yuan Xuan, Fuel, 378, 132886, 2024

[11] Designing High-Performance Fuels through Graph Neural Networks for Predicting Cetane Number of Multicomponent Surrogate Mixtures; Yeonjoon Kim*, **Sabari Kumar***, Jaeyoung Cho, Nimal Naser, Wonjong Ko, Peter C. St. John, Robert L. McCormick, Seonah Kim, SAE Technical Paper No. 2023-32-0052, 2023 (Stars indicate equal contribution)

[12] Physics-informed Graph Neural Networks for Predicting Cetane Number with Systematic Data Quality Analysis; Yeonjoon Kim, Jaeyoung Cho, Nimal Naser, **Sabari Kumar**, Keunhong Jeong, Robert L. McCormick, Peter C. St. John, Seonah Kim, Proc. Comb. Inst., 39, 4, 4969-4978, 2022

Posters

[1] **Sabari Kumar**, Olivia Harman, Seonah Kim. Topoformer: Predicting Protein Solubilities Using Geometric and Toplogical Information. Presented at the Fall 2024 American Chemical Society COMP and SciMix Poster Sessions, Denver, CO

[2] **Sabari Kumar**, Seonah Kim. Predicting Protein Solubilities Using Geometric and Toplogical Information. Presented at the Fall 2023 American Chemical Society COMP and SciMix Poster Sessions, San Fransisco, CA

[3] **Sabari Kumar**, Yeonjoon Kim, Shree Sowndarya Santhanalakkshmi Vejaykummar, Peter St. John, Robert S. Paton, Seonah Kim. Predicting Ring Opening Bond Dissociation Enthalpies from 2D Molecular Structures. Presented at the 2022 Houk Research Conference, University of California Los Angeles.

[4] **Sabari Kumar**, Yeonjoon Kim, Shree Sowndarya Santhanalakkshmi Vejaykummar, Peter St. John, Robert S. Paton, Seonah Kim. Towards Predicting Ring Opening Bond Dissociation Enthalpies from 2D Molecular Structures. Presented at the Spring 2022 American Chemical Society COMP and SciMix Poster Sessions, San Diego, CA.

Invited Talks

[1] **Sabari Kumar**, Applications of Topological Data Analysis in Computational Chemistry. Presented at the Colorado State Univeristy Department of Mathematics Applied Topology Seminar Series, November 29, 2022

Professional Activities

- Organizer and Curriculum Developer, Computation Boot Camp, NSF Center for Sustainable Photoredox Catalysis, 2025
- Graduate Student Representative, Climate and Culture Working Group, Dept. of Chemistry, Colorado State University, 2024-2025
- Co-President, Chemistry Graduate Student Organization, Colorado State University, 2023-2024
- Organizer and Lecturer, Linear Algebra for Computational Chemistry and Data Science, Colorado State University Theoretical Chemistry Group, Spring 2024
- Guest Lecturer, CHEM571A, Quantum Chemistry, Colorado State University, Fall 2023
- Guest Speaker, 'An Introduction to Molecular Dynamics Using OpenMM', CHEM578B Computational Chemistry (Molecular Dynamics), Colorado State University, Spring 2023
- Organizer, Colorado State University Theoretical Chemistry Group Coding Camp, Summer 2022
- Volunteer, Science Education, Irish Elementary Escuela Bilingüe, Fort Collins, CO 2021-2022

References

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[3] Dr. Yeonjoon Kim, Assistant Professor
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[4] Dr. Fabian Thiemann, Research Scientist
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