Viraj D. Gandhi, PhD

Home address:
2037 S. College Street, Apt 503,
Auburn, AL 36832
Ph: (860) 371-0388

Work Address:
354 Mell St, Suite 273
Auburn, AL 36832
Ph: (334) 844-4043

Research interest

Thermofluid systems and transport phenomena across molecular and continuum scales; computational fluid dynamics (CFD) and multi-physics modeling; system-level analysis and design; ion mobility and mass spectrometry; fluid-based sensing and detection systems; heat and mass transfer in engineering applications.

Research Appointments

Auburn University – Postdoctoral Researcher / Instrumentation Engineer *Jan-2025 to current*

- Lead the development, commissioning, and operation of a SLIM-based ion mobility spectrometer for advanced particle detection
- Design and optimize ion transport systems using computational tools, including CFD and ion trajectory simulations (SIMION)
- Develop MATLAB-based tools for data processing and analysis of ion mobility experiments
- Diagnose and resolve system-level challenges related to ion transmission, field effects, and vacuum conditions
- Ensure reliable and reproducible system performance through calibration, validation, and system optimization
- Collaborate with interdisciplinary teams to integrate experimental and computational components

Purdue University – Graduate Research Assistant *Sept-2019 to May-2024*

- Designed and developed a custom DMA-MS platform, including vacuum interfaces and ion-optical components
- Established experimental and computational workflows for ion mobility and mass spectrometry analysis of molecular systems
- Performed CFD simulations to improve transport and capture efficiency in DESI-MS systems
- Identified and resolved performance limitations in mass spectrometry systems related to calibration and signal stability
- Improved predictive accuracy of ion mobility models by ~22% through refined ion–gas interaction modeling
- Developed molecular dynamics-based methods to characterize protein structures in the gas phase

Education

Ph.D. in Mechanical Engineering **GPA: 3.97/4.00**
Purdue University, West Lafayette, IN *May – 2024*

- Dissertation: Theoretical and numerical prediction of ion mobility for flexible all-atom structures under arbitrary fields and subject to structural rearrangement. An initial probing into the effects of internal degrees of freedom.
- Advisor: Dr. Carlos Larriba-Andaluz

M.S. in Mechanical Engineering **GPA: 3.97/4.00**

Purdue University, Indianapolis, IN *August – 2019*

- Dissertation: Parametric designs and weight optimization using direct and indirect aero-structure load transfer methods.
- Advisor: Dr. Hamid Dalir

B.S. in Mechanical Engineering **Grade: Distinction**

Pandit Deendayal Petroleum University, Gandhinagar, Gujarat, India *June – 2017*

Teaching Experience

Purdue University – Undergraduate Research Mentor *Aug-2022 to May-2024*

- Co-mentored undergraduate students on research projects related to fluid and thermal systems
- Guided students in problem formulation, data analysis, and presentation of results
- Supported students in developing research posters and communicating technical findings

Purdue University – TA - Mechanical Engineering Laboratories *Aug-2020 to May-2022*

- Supported laboratory instruction in heat transfer, dynamics, vibrations, and statics
- Guided students through experimental procedures, data analysis, and interpretation of results
- Assisted in troubleshooting experimental setups and reinforcing the connection between theory and observation
- Facilitated discussions to improve student understanding of engineering concepts and experimental methods

Purdue University – Instructor (Problem-Solving Sessions) – Fluid Mechanics *Jan-2020 to May-2020*

- Led problem-solving sessions, guiding students to reason through fluid behavior before formal derivations
- Encouraged active participation by asking students to predict outcomes and discuss underlying physical principles
- Reinforced connections between theoretical concepts and practical applications

Teaching interests

- Thermodynamics
- Fluid Mechanics
- Heat Transfer
- Engineering Computation and Modeling
- Mechanical Engineering Laboratories
- Senior Design

Published manuscripts

(from Google Scholar: Citations = 214; h-index = 9; i10 index = 7)

1. Latif, M.; Chen, X.; Gandhi, V. D.; Hua, L.; Clowers, B.; Larriba-Andaluz, C. Stepwise Optimization of Traveling Wave Profiles and Inverse Gating Pattern in Structure for Lossless Ion Manipulation Platform. *International Journal of Mass Spectrometry* **2025**, 117420.
2. Lee, J. Y.; Gandhi, V. D.; Harrilal, C.; Parvate, A. D.; Ives, A.; Bhotika, H.; Thibert, S. M.; Zhang, X.; Schenter, G. K.; Larriba-Andaluz, C. Characterization of Gas-Phase Native (-like) Proteins Using Structures for Lossless Ion Manipulations. *Analytical Chemistry* **2025**.
3. Wilson, S.; Li, X.; Gandhi, V. D.; Johnson, A.; Schreiber, E.; Ryan, L.; Sertse, L.; Larriba-Andaluz, C.; Matson, E. M.; Laskin, J. Unraveling Ligand-Driven Isomerism in Redox-Active Mixed-Ligand Polyoxometalates Using Ion Mobility Spectrometry. *ACS nano* **2025**, *19* (44), 38544-38552.
4. Gandhi, V. D.; Mubas-Sirah, F.; Latif, M.; Hua, L.; Tootchi, A.; Larriba-Andaluz, C. Ion mobility calculations of flexible all-atom systems at arbitrary fields using two-temperature theory. *Physical Chemistry Chemical Physics* **2024**, *26* (5), 4118-4124.
5. Gandhi, V. D.; Hua, L.; Lawrenz, M.; Latif, M.; Rolland, A. D.; Campuzano, I. D.; Larriba-Andaluz, C. Elucidating Protein Structures in the Gas Phase: Traversing Configuration Space with Biasing Methods. *Journal of Chemical Theory and Computation* **2024**, *20* (21), 9720-9733.
6. Gandhi, V. D.; Hua, L.; Chen, X.; Latif, M.; Larriba-Andaluz, C. A Critical Review of the two-temperature theory and the derivation of matrix elements. High field Ion mobility and energy calculation for all-atom structures in light gases using a 12-6-4 potential. *Talanta Open* **2023**, 100191.
7. Gandhi, V. D.; Lee, J.; Hua, L.; Latif, M.; Hogan, C. J.; Larriba-Andaluz, C. Investigation of Zero-/High-Field Ion Mobility Orthogonal Separation Using a Hyphenated DMA–FAIMS System and Validation of the Two-Temperature Theory at Arbitrary Field for Tetraalkylammonium Salts in Nitrogen. *Analytical Chemistry* **2023**.
8. Chen, X.; Newsome, G. A.; Buchanan, M.; Glasper, J.; Hua, L.; Latif, M.; Gandhi, V. D.; Li, X.; Larriba-Andaluz, C. Flow-Optimized Model for Gas Jet Desorption Sampling Mass Spectrometry. *The Journal of Physical Chemistry A* **2023**, *127* (5), 1353-1359.
9. Gandhi, V. D.; Short, K.; Hua, L.; Rodríguez, I.; Larriba-Andaluz, C. A numerical tool to calculate ion mobility at arbitrary fields from all-atom models. *Journal of Aerosol Science* **2022**, 106122.
10. Chen, X.; Latif, M.; Gandhi, V. D.; Chen, X.; Hua, L.; Fukushima, N.; Larriba-Andaluz, C. Enhancing separation and constriction of ion mobility distributions in drift tubes at atmospheric pressure using varying fields. *Analytical Chemistry* **2022**, *94* (14), 5690-5698.
11. Latif, M.; Chen, X.; Gandhi, V. D.; Larriba-Andaluz, C.; Gamez, G. Field-Switching Repeller Flowing Atmospheric-Pressure Afterglow Drift Tube Ion Mobility Spectrometry. *Journal of the American Society for Mass Spectrometry* **2022**, *33* (4), 635-648.
12. Gandhi, V. D.; Harrilal, C. P.; Nagy, G.; Chen, X.; Buchanan, M. G.; Wojcik, R.; Conant, C. R.; Donor, M. T.; Ibrahim, Y. M.; Garimella, S. V. Measurement and Theory of Gas-Phase Ion Mobility Shifts Resulting from Isotopomer Mass Distribution Changes. *Analytical Chemistry* **2021**, *93* (45), 14966-14975.

13. Gandhi, V. D.; Larriba-Andaluz, C. Predicting ion mobility as a function of the electric field for small ions in light gases. *Analytica Chimica Acta* **2021**, *1184*, 339019.
14. Vicent, C.; Martinez-Agramunt, V.; Gandhi, V. D.; Larriba-Andaluz, C.; Gusev, D. G.; Peris, E. Ion mobility mass spectrometry uncovers guest-induced distortions in a supramolecular organometallic metallosquare. *Angewandte Chemie* **2021**, *133* (28), 15540-15545.
15. Gandhi, V. D.; Joe, J.; Dannenhoffer, J. F.; Dalir, H. Rapid design generation and multifidelity analysis of aircraft structures. *Aerospace Science and Technology* **2021**, *112*, 106612.
16. Coots, J.; Gandhi, V. D.; Onakoya, T.; Chen, X.; Andaluz, C. L. A parallelized tool to calculate the electrical mobility of charged aerosol nanoparticles and ions in the gas phase. *Journal of Aerosol Science* **2020**, 105570.
17. Chen, X.; Gandhi, V. D.; Coots, J.; Fan, Y.; Xu, L.; Fukushima, N.; Larriba-Andaluz, C. High resolution varying field drift tube ion mobility spectrometer with diffusion autocorrection. *Journal of Aerosol Science* **2020**, *140*, 105485.

Conference Presentations

(† denotes the presenter; oral if underlined)

1. Viraj D. Gandhi, Kimberly Y. Kartowikromo, Gordon A. Anderson, Aneesh Prabhakaran, Iffat Jerin, and Ahmed M. Hamid, "Development of a portable SLIM-Based ion-mobility platform for trace-level detection", American Chemical Society national meeting, Atlanta, GA, March 2026.
2. Viraj D. Gandhi, Kimberly Y. Kartowikromo, Gordon A. Anderson, Aneesh Prabhakaran, Iffat Jerin, and Ahmed M. Hamid, "Development of a Portable SLIM-Based Ion Mobility Platform for Trace-Level Detection", Southeastern and Southwest Regional Meeting, Orlando, FL, October 2025.
3. Viraj D. Gandhi, Kimberly Y. Kartowikromo, Gordon A. Anderson, Aneesh Prabhakaran, and Ahmed M. Hamid, "Design and Optimization of a Structures for Lossless Ion Manipulations (SLIM)-Based Ion Mobility Spectrometer for Environmental and Clinical Applications", American Society of Mass Spectrometry 73rd annual meeting, Baltimore, MD, June 2025.
4. Viraj D. Gandhi and Carlos Larriba-Andaluz, "Characterizing gas-phase protein structures using ion-mobility mass spectrometry and adaptive biased molecular dynamics, through solvent accessible-surface guided compaction", American Society of Mass Spectrometry 73rd annual meeting, Baltimore, MD, June 2025
5. Viraj D. Gandhi, Morgan Lawrenz, Iain D. G. Campuzano, and Carlos Larriba-Andaluz, "Accurate Characterization of Protein Structures in the Gas Phase: Combining Ion Mobility, Molecular Dynamics Simulations, and Enhanced Energy Landscape Sampling Methods", International Society for Ion Mobility Spectrometry, Miami, Florida, July 2024
6. Viraj D. Gandhi, Morgan Lawrenz, Iain D. G. Campuzano, and Carlos Larriba-Andaluz, "Characterizing Gas-Phase Protein Structures Using Ion Mobility–Mass Spectrometry and Adaptive Biased Molecular Dynamics", American Society of Mass Spectrometry 72nd annual meeting, Anaheim, CA, June 2024
7. Viraj D Gandhi, Jung Yun Lee, Christopher Harrilal, Amar D Parvate, Harsh Bhotika, Carlos Larriba-Andaluz, James E Evans, Yehia M Ibrahim, Sandilya VB Garimella, "Molecular Dynamic Studies of Protein-Surface Interactions During SLIM Enabled Mobility-Selective Ion Soft-Landing", ASMS 38th

Asilomar Conference on New Frontiers in Ion Mobility-Mass Spectrometry from Applications to Instrumentation, Pacific Grove, CA, October 2024

8. Viraj D. Gandhi; Jihyeon Lee; Christopher J Hogan Jr.; Carlos Larriba-Andaluz, "Investigating the Effect of High-Field Inelastic Collisions Using a DMA-FAIMS Hybrid Method for Improved Ion Mobility Characterization", American Society of Mass Spectrometry 71st annual meeting, Houston, TX, June 2023
9. Viraj D. Gandhi, Leyan Hua and Carlos Larriba-Andaluz, "Protein Compaction in the Gas Phase Studied by Ion Mobility–Mass Spectrometry and Adaptive Biased Gas-Phase Molecular Dynamics Simulations", European Aerosol Conference, Malaga, Spain, September 2023
10. Viraj D. Gandhi, Xuemeng Chen, Leyan Hua, Carlos Larriba-Andaluz, "Predicting Ion Mobility by Including Non-Linear Effects of High Electric Field Strength, Inelasticity of Collisions, and Internal Degrees of Freedom", International Society for Ion Mobility Spectrometry, Memphis, Tennessee, July 2022
11. Viraj D. Gandhi; Xuemeng Chen; Mohsen Latif; Xi Chen; Leyan Hua; Carlos Larriba-Andaluz, "Predicting Ion Mobility in Electric Fields of Arbitrary Strength: Higher-Order Approaches and Essential Data", American Society of Mass Spectrometry 70th annual meeting, Minneapolis, MN, June 2022
12. Viraj D. Gandhi and Carlos Larriba-Andaluz, "Prediction of Ion Mobility at High E/N Using the Two-Temperature Theory to Maximize Selectivity", American Association for Aerosol Research, Virtual (Covid), 2021
13. Viraj D. Gandhi, Christopher P. Harrilal, Gabe Nagy, Xi Chen, Sandilya Garimella, Richard D. Smith, Carlos Larriba-Andaluz, "Numerical Description of Isotopomer Ion Mobility Separations Based on Mass Distribution Effects on Ion Rotation", American Society of Mass Spectrometry 69th annual meeting, Philadelphia, PA, November 2021
14. Viraj D. Gandhi, Jayden Pothoof, Carlos Larriba-Andaluz, "The Effect of Potential Interaction and Atomic Mass on the Nature of Gas–Surface Scattering and Accommodation of Charged Particles: Transitioning from Specular to Diffuse Reemission", American Association for Aerosol Research, Virtual (Covid), 2020
15. Viraj D. Gandhi and Carlos Larriba-Andaluz, "Deviations from the Mason–Schamp Equation for Small Molecules: An Ion Mobility Study" , American Society of Mass Spectrometry 70th annual meeting, Virtual (Covid), 2020
16. Viraj D. Gandhi, John Joe, John F. Dannenhoffer III, Hamid Dalir, "Rapid Generation of Parametric Aircraft Structural Models", American Institute of Aeronautics and Astronautics, San Diego, California, January 2019

Presentations from submitted and accepted abstracts

1. Jung Lee; Viraj D. Gandhi; Christopher Harrilal; Amar Parvate; Stephanie M. Thibert; Ashley Ives; Xin Zhang; Gregory K Schenter; Carlos Larriba-Andaluz; James E Evans; Yehia M. Ibrahim; Sandilya Garimella, "Study of Conformational Space for Native(-Like) Proteins Using Multi-Pass Separations in Structures for Lossless Ion Manipulations and Molecular Dynamics Simulations", American Society of Mass Spectrometry 73rd annual meeting, Baltimore, MD, June 2025
2. Jung Lee; Viraj D. Gandhi; Christopher Hariilal; Amar Parvate; Stephanie M. Thibert; Ashley Ives; Xin Zhang; Gregory K Schenter; Yehia M. Ibrahim; Carlos Larriba-Andaluz; James E Evans; Sandilya

Garimella, “Mobility and Mass Selective Isolation, Separation, and Characterization of Macro-Biomolecules”, American Society of Mass Spectrometry 73rd annual meeting, Baltimore, MD, June 2025

3. Xilai Li; Shana Havenridge; Solita Wilson; Viraj D. Gandhi; Carlos Larriba-Andaluz; Cong Liu; Julia Laskin. “Unraveling the Structures of Transition-Metal Nanoclusters with Ion Mobility–Mass Spectrometry and Computational Modeling”, American Society of Mass Spectrometry 73rd annual meeting, Baltimore, MD, June 2025
4. Mohsen Latif; Viraj D. Gandhi; Leyan Hua; Carlos Larriba-Andaluz, “Investigation of the Effects of Traveling-Wave Profiles in SLIM”, American Society of Mass Spectrometry 72nd annual meeting, Anaheim, CA, June 2024
5. Farah Mubas-Sirah; Viraj D. Gandhi; Mohsen Latif; Leyan Hua; Amirreza Tootchi; Carlos Larriba-Andaluz, “Ion Mobility Calculations of Flexible All-Atom Systems at Arbitrary Fields Using Two-Temperature Theory”, American Society of Mass Spectrometry 72nd annual meeting, Anaheim, CA, June 2024
6. Amirreza Tootchi; Viraj D. Gandhi; Farah Mubas-Sirah; Carlos Larriba-Andaluz, “Ion Mobility Separation by means of Space Charge in Accumulation Regions with high concentrations”, American Society of Mass Spectrometry 72nd annual meeting, Anaheim, CA, June 2024
7. Carlos Larriba-Andaluz and Viraj D. Gandhi, “Ion–Gas Collisional Energy Transfer Between Internal Degrees of Freedom”, American Society of Mass Spectrometry 72nd annual meeting, Anaheim, CA, June 2024
8. Leyan Hua, Viraj D. Gandhi, Carlos Larriba-Andaluz, “Elucidation of denatured protein structures through Ion Mobility Spectrometry Mass Spectrometry by comparison to Gas Phase Ion Structures of homopolymers”, American Society of Mass Spectrometry 71st annual meeting, Houston, TX, June 2023
9. Xuemeng Chen; Viraj D. Gandhi; Heikki Junninen; Carlos Larriba-Andaluz, “Characterization Study of Ion Mobility of Small Bio-Analyte Ions in Positive and Negative Modes”, American Society of Mass Spectrometry 70th annual meeting, Minneapolis, MN, June 2022
10. Xi Chen; Mohsen Latif; Viraj D. Gandhi; Xuemeng Chen; Leyan Hua; Carlos Larriba Andaluz, “Enhancing Separation and Constriction of Ion Mobility Distributions in Drift Tubes at Atmospheric Pressure Using Varying Fields”, American Society of Mass Spectrometry 70th annual meeting, Minneapolis, MN, June 2022
11. Cameron N. Naylor, Christoph Schaefer, Viraj D. Gandhi, Ansgar T. Kirk, Carlos Larriba-Andaluz, Stefan Zimmermann, “Elucidating the Ionization Mechanism of Aniline Isomers by Combining HiKE-IMS with Ion Mobility Simulations”, American Society of Mass Spectrometry 70th annual meeting, Minneapolis, MN, June 2022
12. Carlos Larriba-Andaluz and Viraj D. Gandhi, “The Study of Inelastic Collisions in Electrical Mobility by Coupling MD to Kinetic Theory Physical Gas Modelling”, American Association for Aerosol Research, Virtual (Covid), 2021
13. Carlos Larriba-Andaluz and Viraj D. Gandhi, “Inadequacies of Common Theoretical and Numerical Tools to Predict Ion Mobilities on Par with High-Resolution Experimental Observations and How to Overcome Them”, American Society of Mass Spectrometry 70th annual meeting, Virtual (Covid), 2020

Honors and awards

Best poster presentation, Asilomar ASMS conference	2024
Travel grant, Asilomar ASMS conference	2024
Graduate student travel award, ASMS conference	2023
Student travel award, ISIMS conference	2021
Student scholarship, ASMS	2021
University travel grant, IUPUI	2021
Graduate student travel grant, Graduate and Professional Organization	2021
AFRL full scholarship, Airforce Research Lab	2018

Services

Reviewer: *Int. J. Mass Spec., Scientific Reports, Aerosol Science and Technology, Plos One*

Session chair: European Aerosol Conference (2023), International Society for Ion Mobility Spectrometry (2021)

References

1. Dr. Carlos Larriba-Andaluz
   Associate Professor of Mechanical Engineering
   Purdue University, West Lafayette, IN
   Email: clarriba@purdue.edu
   Phone: 317-274-8993

2. Dr. Sandilya V.B. Garimella
   Computational Scientist
   Pacific Northwest National Laboratory
   Email: sandilya.garimella@pnnl.gov
   Phone: 509-371-6326

3. Dr. Henry Benner
   Founder, CTO
   ionDX
   Email: hbenner@iondx.com
   Phone: 925-708-4171