

Amartya S. Banerjee

Contact Information

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Education

- **Ph.D.** in Aerospace Engineering & Mechanics, December 2013
University of Minnesota, Minneapolis, USA.
Advisors: Richard D. James and Ryan S. Elliott.
- **M.S.** in Aerospace Engineering & Mechanics, November 2011
University of Minnesota, Minneapolis, USA.
- **M.S.** in Mathematics, April 2011
University of Minnesota, Minneapolis, USA.
- **B.Tech. (Honors)** in Aerospace Engineering, August 2007
Indian Institute of Technology (IIT), Kharagpur, India.

Professional Appointments

- **Assistant Professor:** Department of Materials Science and Engineering, University of California, Los Angeles, USA (July 2019 – present).
- **Assistant Professor:** Mechanical, Aerospace and Biomedical Engineering, University of Tennessee, Knoxville, USA (August 2018 – June 2019).
- **Postdoctoral Fellow:** Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, USA (June 2015 – July 2018).
Mentors: Lin Lin and Chao Yang.
- **Postdoctoral Associate:** Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, USA (January 2014 – May 2015).
- **Graduate Research Assistant:** Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, USA (2008 – 2013).
- **Graduate Teaching Assistant:** Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, USA (Fall 2007).
- **Undergraduate Intern:** Smart Materials and MEMS Laboratory, University of Arkansas at Little Rock, Little Rock, Arkansas, USA (May – July, 2006).
Mentor : Abhijit Bhattacharyya.
- **Undergraduate Intern:** Low Turbulence Wind Tunnel Laboratory, Indian Institute of Science, Bangalore, India (May – July, 2005).
Mentor : Jyotirmoy Dey.

Research Interests

- **First principles (quantum mechanical) methods** for the **design, discovery and characterization of novel materials and structures**. Extending the scope of first principles methods for applications to problems in mechanics (e.g. studies of materials defects), simulations of Compositionally Complex / High Entropy Alloys and simulations of molecules of importance in biology.
- Applications of **Data Science/Machine Learning** techniques to materials science problems.
- **Usage of symmetry principles** in various areas of science and engineering, including:
 - Investigation of **Chiral/twisted materials** with strongly correlated electronic states / anomalous transport properties.
 - Usage of the **Objective Structures framework** for the exploration and systematic study of unprecedented nano-materials, nano-structures and their deformations.
 - **Reduction of scientific computation problems / design of computational solvers.**

- **Simulations of quantum materials, energy materials.**
- **Multi-scale methods and algorithms** for the study of defects in materials – design, analysis and implementation.
- **Mechanics of materials and structures, solid mechanics.**
- **Numerical analysis and scientific computation** (spectral methods, non-linear PDEs, numerical linear algebra, high performance computing).

Honors and Awards

- Faculty Career Development Award, 2022.
University of California, Los Angeles.
- US Junior Oberwolfach Fellowship, 2013.
(Supported by the U.S. National Science Foundation.)
- John A. & Jane Dunning Copper Fellowship, 2008.
University of Minnesota, Minneapolis, USA.
- Summer Fellowship, 2008.
University of Minnesota, Minneapolis, USA.
- Best B.Tech Project, 2007.
Indian Institute of Technology, Kharagpur, India, 2007.

Publications and Preprints

(underlined = Member of Banerjee's Ab Initio Simulations Lab at UCLA, * = corresponding author)

Published journal articles:

- S. Pathrudkar, S. Taylor, A. Keripale, A. S. Gangan, P. Thiagarajan, S. Agarwal, J. Marian, S. Ghosh and **A.S. Banerjee***: Electronic structure prediction of medium and high entropy alloys across composition space (2025); *Accepted manuscript, npj Computational Materials* ([arXiv](#)).
- S. Pathrudkar, P. Thiagarajan, S. Agarwal, **A.S. Banerjee*** and S. Ghosh (2024): Electronic Structure Prediction of Multi-million Atom Systems Through Uncertainty Quantification Enabled Transfer Learning (2024); *npj Computational Materials*, Volume 10, 175 (Links: [Journal](#), [pdf](#))
- Md. T. Ahmed, C. Wang, **A.S. Banerjee** and N. Admal (2024): Bicrystallography-informed Frenkel-Kontorova model for interlayer dislocations in strained 2D heterostructures; *Mechanics of Materials*, Volume 190, 104903 (Links: [Journal](#), [pdf](#)).
- H. M. Yu, S. Sharma, O. Liebman, S. Agarwal and **A.S. Banerjee*** (2023): Carbon Kagome Nanotubes — quasi-one-dimensional nanostructures with flat bands; *RSC Advances*; 2024, 14, 963-981 (Links: [Journal](#), [pdf](#))
- S. Agarwal and **A.S. Banerjee*** (2023): Solution of the Schrödinger equation for quasi-one-dimensional materials using helical waves; *Journal of Computational Physics*; Volume 496, 112551 (Links: [Journal](#), [pdf](#)).
- S. Agarwal, D. R. Kattnig, C. D. Aiello and **A.S. Banerjee*** (2023): The Biological Qubit: Calcium Phosphate Dimers, Not Trimers; *The Journal of Physical Chemistry Letters*; 14, 2518-2525 (Links: [Journal](#), [pdf](#))
- S. Pathrudkar, H. M. Yu, S. Ghosh and **A.S. Banerjee*** (2022): Machine learning based prediction of the electronic structure of quasi-one-dimensional materials under strain *Physical Review B*; Volume 105, No. 19, 195141 (Links: [Journal](#), [pdf](#))
- C. D. Aiello, J. Abendroth, M. Abbas, A. Afanasev, S. Agarwal, **A. S. Banerjee**, D. Beratan, J. N. Belling, et al. (2022): A Chirality-Based Quantum Leap: A Forward-Looking Review; *ACS Nano*; 16, 4, 4989-5035 (Links: [Journal](#), [pdf](#)) [Article featured as ACS Editors' Choice]
- H. M. Yu and **A.S. Banerjee*** (2022): Density functional theory method for twisted geometries with application to torsional deformations in group-IV nanotubes; *Journal of Computational Physics*; Volume 456, 111023 (Links: [Journal](#), [pdf](#))
- S. Agarwal, C. D. Aiello, D. R. Kattnig and **A.S. Banerjee*** (2021): The Dynamical Ensemble of the Posner Molecule is not Symmetric; *The Journal of Physical Chemistry Letters*; 12, 10372 - 10379 (Links: [Journal](#), [pdf](#))

- **A.S. Banerjee*** (2021): Ab initio framework for systems with helical symmetry: theory, numerical implementation and applications to torsional deformations in nanostructures; *Journal of the Mechanics and Physics of Solids*; Volume 154, 104515 (Links: [Journal](#), [pdf](#))
- S. Ghosh, **A.S. Banerjee** and P. Suryanarayana (2019): Symmetry-adapted real-space density functional theory for cylindrical geometries: Application to large group-IV nanotubes; *Physical Review B*; Volume 100 (Issue 12), 125143 (Links: [Journal](#), [pdf](#))
- **A.S. Banerjee**, L. Lin, P. Suryanarayana, C. Yang and J.E. Pask (2018): Two-level Chebyshev filter based complementary subspace method: pushing the envelope of large-scale electronic structure calculations; *Journal of Chemical Theory and Computation*; Volume 14 (6), Pages 2930–2946 (Links: [Journal](#), [pdf](#))
- W. Hu, L. Lin, **A.S. Banerjee**, E. Vecharynski and C. Yang (2017): Adaptively Compressed Exchange Operator for Large Scale Hybrid Density Functional Calculations with Applications to the Adsorption of Water on Silicene; *Journal of Chemical Theory and Computation*; Volume 13 (3), Pages 1188–1198 (Links: [Journal](#), [pdf](#))
- **A.S. Banerjee**, L. Lin, W. Hu, C. Yang and J.E. Pask (2016): Chebyshev polynomial filtered subspace iteration in the Discontinuous Galerkin method for large-scale electronic structure calculations; *The Journal of Chemical Physics*; Volume 145 (15), 154101 (Links: [Journal](#), [pdf](#))
- **A.S. Banerjee** and P. Suryanarayana (2016): Cyclic Density Functional Theory : A route to the first principles simulation of bending in nanostructures; *Journal of the Mechanics and Physics of Solids*; Volume 96, Pages 605–631 (Links: [Journal](#), [pdf](#))
- **A.S. Banerjee**, P. Suryanarayana and J.E. Pask (2016): Periodic Pulay method for robust and efficient convergence acceleration of self-consistent field iterations; *Chemical Physics Letters*; Volume 647, Pages 31–35 (Links: [Journal](#) , [pdf](#))
- **A.S. Banerjee**, R. S. Elliott and R. D. James (2015): A spectral scheme for Kohn-Sham density functional theory of clusters. *Journal of Computational Physics*; Volume 287, Pages 226–253 (Links: [Journal](#) , [pdf](#))
- **A.S. Banerjee**, A.C. Mandal and J. Dey (2006): Particle image velocimetry studies of an incipient spot in the Blasius boundary layer. *Experiments in Fluids*; Volume 40 (6), Pages 928–941 (Links: [Journal](#) , [pdf](#))

Submitted manuscripts and preprints:

- C. Wang, C. J. Garcia-Cervera and **A. S. Banerjee***: Bloch Oscillations and Landau-Zener Transitions in Flat-Band Lattices with Quadratic and Linear Band Touchings (2025); *Submitted* ([arXiv](#))
- Md. T. Ahmed, C. Wang, **A. S. Banerjee** and N. C. Admal: Multiscale analysis of large twist ferroelectricity and swirling dislocations in bilayer hexagonal boron nitride (2025); *Submitted* ([arXiv](#))
- S. Hossain, P. Thiagarajan, S. Pathrudkar, S. Taylor, A. S. Gangan, **A.S. Banerjee*** and S. Ghosh: Surprisingly High Redundancy in Electronic Structure Data (2025); *Submitted* ([arXiv](#))
- S. Sharma, C. Wang, H.M. Yu, and **A.S. Banerjee***: Electronic states and mechanical behaviors of phosphorus carbide nanotubes — structural and quantum phase transitions in a quasi-one-dimensional material (2024); *Submitted* ([arXiv](#)).
- S. Sharma and **A.S. Banerjee***: Strain-Tunable Topological Phase Transitions in Line- and Split-Graph Flat-Band Lattices (2024); *Submitted* ([arXiv](#)).

Theses

- **A.S. Banerjee** (2013): Density Functional Methods for Objective Structures: Theory and Simulation Schemes. *Ph.D. Thesis*; University of Minnesota, Minneapolis, USA. ([Link](#))
- **A.S. Banerjee** (2011): Harmonic analysis on isometry groups of Objective Structures and its applications to Objective Density Functional Theory. *M.S. Thesis*; University of Minnesota, Minneapolis, USA.
- **A.S. Banerjee** (2007): Numerical simulation studies on cavity flows. *Undergraduate Thesis*; Indian Institute of Technology, Kharagpur, India.

Scientific Software

- S. Agarwal and **A.S. Banerjee** (2024): HelicES (Helical Electronic Structure) — a MATLAB package for electronic structure calculations of nanomaterials with helical and cyclic symmetries. ([Link](#))
- L. Lin, C. Yang, W. Hu, W. Jia, **A.S. Banerjee** and D. Williams-Young (2021): Scalable Electronic Structure (ScalES) v1.0 (Open source, large scale electronic structure calculation software based on the Discontinuous Galerkin method, developed under DOE's SciDAC program: ([Link](#)))

Invited Talks

(At Workshops/Conferences, Schools, Universities & Research Labs)

- **2025:**
 - Department of Materials, University of California, Santa Barbara, California, USA (May, 2025).
 - U.S. Association for Computational Mechanics (USACM) Thematic Workshop on “Emerging Trends in Nanomechanics: Experimental, Computational and Machine Learning Approaches”, University of Illinois, Urbana-Champaign, USA (September, 2025).
- **2024:**
 - Materials Research Society (MRS) Spring Meeting (April, 2024), Seattle, Washington, USA.
 - Science Academy STEM Talk (April, 2024) — quantum physics themed popular science talk delivered to over 400 middle and high-school students. The Science Academy STEM Magnet, North Hollywood, California, USA.
 - Institute for Advanced Study, The Hong Kong University of Science and Technology, Focused Program on Continuum Theory and Mathematical Modeling of Phase Transition Materials, March 2024 [Delivered via Zoom].
- **2023:**
 - Advances in Computational Mechanics (ACM) conference (October, 2023), Austin, Texas, USA.
 - SoCal Solids Conference, University of Southern California, Los Angeles, USA (September, 2023).
 - March Meeting of the American Physical Society, Las Vegas, Nevada, USA (March, 2023).
- **2022:**
 - Modeling and simulation Tech Forum, 3M, Minneapolis, Minnesota, USA (September, 2022).
 - Workshop on Large-Scale Certified Numerical Methods in Quantum Mechanics, Institute for Pure and Applied Mathematics (IPAM), University of California, Los Angeles; Los Angeles, California, USA (May, 2022).
- **2021:**
 - Department of Mechanical Engineering-Engineering Mechanics, Michigan Technological University, Houghton; Michigan, USA (October, 2021). [Delivered via Zoom due to COVID-19]
 - Department of Aerospace and Mechanical Engineering, University of Southern California, Los Angeles; California, USA (August, 2021). [Delivered via Zoom due to COVID-19]
 - Computational Physics Department, HRL Laboratories, Malibu, California. (May, 2021) [Delivered via Zoom due to COVID-19].
- **2020:**
 - Department of Mechanical Engineering, University of California, Merced; [Delivered via Zoom due to COVID-19] (September, 2020).
 - Institute for Chiral Quantum Materials & Devices Spring Workshop organized by Arizona State University; [Delivered via Zoom due to COVID-19] (May, 2020).
- **2019:**
 - Moore Workshop on “Coherent Spin Physics in Biology”, University of California, Los Angeles; Los Angeles, California, USA (December, 2019).

- Department of Mathematics, University of California, Santa Barbara; Santa Barbara, California, USA (October, 2019).
- *U.S. Association for Computational Mechanics (USACM) Workshop* on “Recent Advances in the Modeling and Simulation of the Mechanics of Nanoscale Materials”, University of Pennsylvania, Philadelphia, USA (August 2019).
- MURI Annual meeting on Revolutionary Advances in Correlated Electron Materials; California Institute of Technology, Pasadena, California, USA (May, 2019).
- Materials Sciences and Technology Division, Oak Ridge National Laboratory; Oak Ridge, Tennessee, USA (January, 2019).
- **2018:**
 - Workshop on “Solving or Circumventing Eigenvalue Problems in Electronic Structure Theory”, at the *ELectronic Structure Infrastructure (ELSI) Conference*, Molecular Sciences Software Institute, Richmond, Virginia, USA (August, 2018).
 - Mini - symposium on “Electronic Structure of Materials” at the *Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical Aspects of Material Science*, Portland, Oregon, USA (July, 2018).
 - Institute for Mathematics and its Applications (IMA); Minneapolis, Minnesota, USA, (June, 2018).
 - Department of Materials Science and Engineering, University of California, Los Angeles; Los Angeles, California, USA (April, 2018).
 - Penn Institute for Computational Science / Department of Mechanical Engineering & Applied Mechanics, University of Pennsylvania; Philadelphia, Pennsylvania, USA (March, 2018).
 - Department of Mechanical Engineering, Massachusetts Institute of Technology; Boston, Massachusetts, USA (March, 2018).
 - Department of Mechanical, Aerospace and Biomedical Engineering, University of Tennessee; Knoxville, Tennessee, USA (February, 2018).
- **2017:**
 - Symposium on “Extending accuracy and scales with emerging computing architectures and algorithms” at the *American Chemical Society (ACS) Annual Fall Meeting*, Washington D.C., USA (August, 2017).
 - Department of Civil and Environmental Engineering, University of California, Davis; Davis, California, USA (May, 2017).
 - Department of Civil and Environmental Engineering, Carnegie Mellon University; Pittsburgh, Pennsylvania, USA (March, 2017).
- **2016:**
 - *U.S. Association for Computational Mechanics (USACM) Thematic Workshop* on “Recent Advances in Computational Methods for Nanoscale Phenomena”, University of Michigan, Ann Arbor, USA (August, 2016).
 - Department of Mechanical and Civil Engineering, California Institute of Technology; Pasadena, California, USA (June, 2016).
 - Mini - symposium on “Mathematics and algorithms for ground state electronic structure theory” at the *Society for Industrial and Applied Mathematics (SIAM) Conference on Mathematical Aspects of Material Science*, Philadelphia, Pennsylvania, USA (May, 2016).
 - Symposium on “Linear and multi-linear methods for electronic structure calculations” at the *87th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM)*, Braunschweig, Germany (March, 2016).
- **2015:**
 - Department of Mechanical Engineering, Massachusetts Institute of Technology; Boston, Massachusetts, USA (April, 2015).

- **2014:**
 - Computational Research Division, Lawrence Berkeley National Laboratory; Berkeley, California, USA (December, 2014).
- **2013:**
 - Mini - workshop on “Inelastic and non-equilibrium material behavior: from atomistic structure to macroscopic constitutive relations” at Mathematisches Forschungsinstitut Oberwolfach, Wolfach, Germany (November, 2013).
 - PRedictive Integrated Structural Materials Science (PRISMS) Center, University of Michigan, Ann Arbor, USA (October, 2013).
 - Workshop on Mathematics and Mechanics in the Search for New Materials, Banff, Alberta, Canada (July, 2013).

Conference Presentations

- 18th U.S. National Congress on Computational Mechanics (July 2025), Chicago, Illinois, USA. [3 contributed presentations].
- March Meeting of the American Physical Society (March, 2025), Anaheim, California, USA [4 contributed presentations].
- 2024 Spring Meeting of the Materials Research Society, (April 2024) Seattle, Washington, USA [contributed presentation].
- March Meeting of the American Physical Society (March, 2024), Minneapolis, Minnesota, USA [contributed presentation].
- 58th Annual Technical Meeting of the Society of Engineering Science, (October, 2023) Minneapolis, Minnesota, USA.
- 17th *U.S. National Congress on Computational Mechanics* (July, 2023) Albuquerque, New Mexico [2 contributed presentations].
- The 11th Annual Mach Conference (April, 2023), Baltimore, Maryland, USA.
- March Meeting of the American Physical Society (March, 2023), Las Vegas, Nevada, USA [4 contributed presentations].
- 57th Annual Technical Meeting of the Society of Engineering Science, College Station, Texas, USA (October, 2022). [2 contributed presentations].
- 10th International Conference on Multiscale Materials Modeling (October 2022). Baltimore, Maryland, USA.
- 19th *U.S. National Congress on Theoretical and Applied Mechanics*, (June 2022) Austin, Texas. [contributed presentation]
- March Meeting of the American Physical Society (March, 2022), Chicago, Illinois, USA [3 contributed presentations].
- 16th U.S. National Congress on Computational Mechanics, (July, 2021), [contributed presentation, delivered via Zoom due to COVID-19].
- Spring Meeting of the Materials Research Society (April, 2021), [contributed presentation, delivered via Zoom due to COVID-19].
- March Meeting of the American Physical Society (March, 2021), [contributed presentation, delivered via Zoom due to COVID-19].
- The 10th International Conference on Multiscale Materials Modeling, Baltimore, Maryland, USA (Scheduled for October 2020) [Cancelled due to COVID-19].
- 56th Annual Technical Meeting of the Society of Engineering Science, St. Louis, Missouri, USA (October, 2019).
- 18th U.S. National Congress for Theoretical and Applied Mechanics, Chicago, Illinois, USA (June, 2018).

- 54th Annual Technical Meeting of the Society of Engineering Science and ASME-AMD joint conference, Boston, Massachusetts, USA (July, 2017).
- 53rd Annual Technical Meeting of the Society of Engineering Science, College Park, Maryland, USA (October, 2016).
- 24th International Conference of Theoretical and Applied Mechanics, Montréal, Canada (August, 2016)
- 52nd Annual Technical Meeting of the Society of Engineering Science, College Station, Texas, USA (October, 2015).
- 13th U.S. National Congress on Computational Mechanics, San Diego, California (July, 2015).
- Materials Research Society – Fall 2014 Meeting & Exhibit, Boston, Massachusetts, USA (December, 2014).
- 51st Annual Technical Meeting of the Society of Engineering Science, West Lafayette, Indiana, USA (October, 2014).
- 17th U.S. National Congress on Theoretical & Applied Mechanics, East Lansing, Michigan, USA (June, 2014).
- 50th Annual Technical Meeting of the Society of Engineering Science and ASME-AMD Annual Summer Meeting, Providence, Rhode Island, USA (July, 2013).
- 12th U.S. National Congress on Computational Mechanics, Raleigh, North Carolina (July, 2013).
- 49th Annual Technical Meeting of the Society of Engineering Science, Atlanta, Georgia, USA (October, 2012).
- 10th World Congress on Computational Mechanics, São Paulo, Brazil (July, 2012).

Other Talks & Presentations

- Panelist on the “Engineer Change: How can engineers work to change the world ?” panel, School of Engineering, UCLA, USA (October 2020) [Participated via Zoom due to COVID-19].
- Journal Club of the Quantum Biology Tech. (QuBiT) Lab at UCLA, California, USA (August 2020) [Delivered via Zoom due to COVID-19] .
- Berkeley/Stanford Computational Mechanics Festival; Berkeley, California, USA (April 2017).
- Lawrence Berkeley National Lab / UC Berkeley Applied Mathematics seminar; Berkeley, California, USA (September 2016).
- Poster presentation at the workshop on Mathematics and Mechanics in the 22nd Century: Seven Decades and Counting; Eugene, Oregon (October, 2015).
- Poster presentation at the Annual Research Exhibition of the Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, USA. (April 2014).
- Research seminar in solid mechanics, Department of Aerospace Engineering & Mechanics, University of Minnesota, Minneapolis, USA. (February 2013).
- Happy Hour of Math seminar (2 lectures) at the Hausdorff Research Institute for Mathematics, Bonn, Germany (May 2012).
- Math-Mechanics research seminar, University of Minnesota, Minneapolis, USA. (March 2012).

Synergistic Activities

- **Proposal Reviewer/Panelist** : National Science Foundation (Mechanics of Materials & Structures program, Condensed Matter and Materials Theory Program), Department of Energy (Basic Energy Sciences program), California NanoSystems Institute.
- **Chair** for Technical Thrust Area committee on “Nanotechnology and Lower Scale Phenomena” for the U.S. Association for Computational Mechanics (USACM) (January 2025 – present) [[Link](#)]; Vice-Chair (January 2022 – December 2024); Member-at-large (January 2020 – 2022).

- **Lead organizer** for U.S. Association for Computational Mechanics (USACM) thematic Workshop on “Data-Driven and Computational Modeling of Materials Across Scales” (May 2023).
Co-organizers: Nikhil Admal (University of Illinois, Urbana-Champaign), Alejandro Strachan (Purdue University), Surya Kalidindi (Georgia Tech.). ([Workshop Website Link](#))
Supported by the NSF under grant # 2325413.
- **Lead organizer** for U.S. Association for Computational Mechanics (USACM) Workshop on “New Trends and Open Challenges in Computational Mechanics: from Nano to Macroscale” (March 2021).
Co-organizers: Nikhil Admal (University of Illinois, Urbana-Champaign), Celia Reina (University of Pennsylvania), Michael Ortiz (Caltech). ([Workshop Website Link](#))
- **Lead organizer** for U.S. Association for Computational Mechanics (USACM) Technical Thrust Area Monthly Webinar Series (Nanotechnology and Lower Scale Phenomena, Summer and Fall 2022).
Co-organizers: Celia Reina (University of Pennsylvania), Anter El-Azab (Purdue University), Jarek Knap (Army Research Lab).
- **Editorial Board Member** : Journal of Materials Science: Materials Theory (2025 – present). ([Link](#))
Handling Editor : MRS Advances (Spring 2021 MRS Meeting Edition).
Reviewer for the journals : Nature Communications, Science Advances, Nanoscale, ACS Nano, Nano Letters, Acta Materialia, Journal of Chemical Theory and Computation, Journal of the Mechanics and Physics of Solids, Journal of Computational Physics, Computer Physics Communications, Applied Physics Letters, Journal of Applied Physics, Journal of Chemical Physics, Journal of Elasticity, Mathematics and Mechanics of Solids, Mechanics Research Communications, International Journal of Solids and Structures, Chemical Physics Letters, SIAM Journal on Scientific Computing, Acta Crystallographica, Journal of Chemical Information and Modeling, Communications in Computational Physics, Computational Condensed Matter, Computational and Structural Biotechnology Journal, RSC Advances, Mathematical Reviews.
- **Co-organizer of the following technical symposia:**
 - “Advances in nanomechanics: computational, experimental and AI-driven approaches” at the 20th U.S. National Congress on Theoretical and Applied Mechanics, Pasadena, California, USA (Upcoming, 2026). Co-organizers: Nikhil Admal (Univ. of Illinois, Urbana Champaign), Susanta Ghosh (Michigan Tech.) and Dibakar Dutta (New Jersey Institute of Technology).
 - “Recent trends in data-driven and computational modeling of materials across scales: from first principles calculations to mesoscale physics” at the 18th U.S. National Congress on Computational Mechanics, Chicago, Illinois, USA. (July 2025).
Co-organizers: Vikram Gavini (Univ. of Michigan) and Susanta Ghosh (Michigan Tech.).
 - “Data-Driven and Multiscale Modeling of Energy and Quantum Materials” at the 17th U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico, USA. (July 2023). Co-organizers: Vikram Gavini (Univ. of Michigan) and Ananya Balakrishna (Univ. of California, Santa Barbara).
 - “Multiscale Mechanics at the Intersection of Theoretical, Computational and Data Driven Approaches” at the Annual Technical Meeting of the Society of Engineering Science, College Station, Texas (October 2022). Co-organizers: Vikram Gavini (Univ. of Michigan).
 - “Quantum Horizons for Computational Mechanics” at the 15th World Congress on Computational Mechanics and 8th Asian Pacific Congress on Computational Mechanics, Yokohama, Japan (August 2022). Co-organizers: Vikram Gavini (Univ. of Michigan), Suvranu De (Rensselaer Polytechnic Institute), Veera Sundararaghavan (Univ. of Michigan), Eiji Tsuchida (National Institute of Advanced Industrial Science and Technology, Japan).
 - “Physics-Based and Data-Driven Multiscale Modeling of Nano-Materials” at the 19th U.S. National Congress on Theoretical and Applied Mechanics, Austin, Texas (June 2022). Co-organizers: Susanta Ghosh (Michigan Technological University), Dibakar Dutta (New Jersey Institute of Technology), Ganesh Balasubramanian (Lehigh University) and Shiva Rudraraju (University of Wisconsin-Madison).
 - “Materials Modeling Across Scales: From First Principles Calculations to Mesoscale Physics” at the 16th U.S. National Congress on Computational Mechanics, Chicago, Illinois (July, 2021). Co-organizers: Vikram Gavini (Univ. of Michigan) and Ananya Balakrishna (Univ. of Southern California).

- “From Quantum Mechanics to Materials Engineering: Recent Progress on the Development and Novel Applications of ab initio Methods in Materials Science” at the 2021 Materials Research Society (MRS) Spring Meeting, Seattle, Washington, USA (April 2021). Co-organizers: Felipe Jornada (Stanford University), Sivan Refaely-Abramson (Weizmann Institute of Science) and Lin Lin (University of California, Berkeley).
- “First Principles Simulations And Their Applications To The Mechanics Of Materials” at the 57th Annual Technical Meeting of the Society of Engineering Science, University of Minnesota, Minneapolis, USA (Scheduled for September, 2020). Co-organizers : Swarnava Ghosh (Caltech) and Phanish Suryanarayana (Georgia Tech.). [Cancelled due to COVID-19]
- “Theory and Simulation of Nanomaterials” at the 56th Annual Technical Meeting of the Society of Engineering Science, Washington University, St. Louis, USA (October, 2019). Co-organizers : Swarnava Ghosh (Caltech) and Phanish Suryanarayana (Georgia Tech.).
- “Modeling at the Intersection of First Principles Methods, Mechanics and Mathematics” at the 15th U.S. National Congress on Computational Mechanics, Austin, Texas (July, 2019). Co-organizers : Vikram Gavini (Univ. of Michigan) and Phanish Suryanarayana (Georgia Tech.).
- “Computational Mechanics at the Atomistic and Electronic Scales” at the 54th Annual Technical Meeting of the Society of Engineering Science, Northeastern University, USA (July, 2017). Co-organizers : Kaushik Bhattacharya (Caltech), Ellad Tadmor (Univ. of Minnesota) and Phanish Suryanarayana (Georgia Tech.).
- “From Quantum Mechanics to Materials Engineering: First Principles Methods in the Mechanics of Materials and Structures” (3 sessions) at the 53rd Annual Technical Meeting of the Society of Engineering Science, University of Maryland, USA (October, 2016). Co-organizers : Co-organizer : Phanish Suryanarayana (Georgia Tech.).
- “First principles methods in the mechanics of materials” (4 sessions) at the 52nd Annual Technical Meeting of the Society of Engineering Science, Texas A & M University, USA (October, 2015). Co-organizer : Phanish Suryanarayana (Georgia Tech.).
- “Recent Progress in Multi-scale Modeling at the Intersection of Ab initio Methods, Mechanics and Mathematics” (6 sessions) at the 13th U.S. National Congress on Computational Mechanics, San Diego, California (July, 2015). Co-organizers : Vikram Gavini (Univ. of Michigan) and Phanish Suryanarayana (Georgia Tech.).
- “Ab initio methods in the Mechanics of Materials” (2 sessions) at the 51st Annual Technical Meeting of the Society of Engineering Science, Purdue University, USA (October, 2014). Co-organizer : Phanish Suryanarayana (Georgia Tech.).

• **Session chair at the following technical symposia :**

- Symposium on “Machine Learning and Simulations” at the 2024 Spring Meeting of the Materials Research Society, Seattle, Washington, USA (April 2024).
- Symposium on “Advances in the Study of Defects through Atomistic / Continuum Coupling Methods” at the 49th Annual Technical Meeting of the Society of Engineering Science, Atlanta, Georgia, USA (October 2012).

• **Organizing and hosting speakers** for the Lawrence Berkeley National Lab / UC Berkeley Applied Mathematics Seminar (Primary host: Prof. Lin Lin, Dept. of Mathematics).

• **Member of the following professional organizations :** American Physical Society (APS), Materials Research Society (MRS), the U.S. Association for Computational Mechanics (USACM), the Society of Engineering Science (SES) and the International Association for Computational Mechanics (IACM).

Other Service Activities

- Graduate Division Faculty Review Committee for the Dissertation Year Award, UCLA (for 2024-2025 academic year recipients).
- Samueli School of Engineering FEC Honors Committee, UCLA (2023).
- Institute for Digital Research and Education (IDRE) Postdoctoral Fellow Selection Committee, UCLA (2021, 2022, 2024).

- Weekly departmental seminar organization, Department of Materials Science & Engineering, UCLA (Spring 2021).
- Graduate Students Admissions Committee, Department of Materials Science & Engineering, UCLA (Fall 2020, 2021, 2022, 2023 and 2024 applicants).
- Ph.D. Preliminary Examination Committee, Department of Materials Science & Engineering, UCLA (Winter 2021, Spring 2024, Fall 2024).
- Graduate Division Faculty Review Committee for the Dissertation Year Fellowship, UCLA (for 2020-2021 academic year recipients).
- Board member, Institute for Digital Research and Education (IDRE), UCLA (July 2020 - current).
- Departmental representative for UCLA's DataX Initiative (Materials Science & Engg. Dept.).
- M.S. Thesis Committee : David Ho (MS&E, UCLA), Yushu Hu (MS&E, UCLA), Ju-Ming Tsai (MS&E, UCLA).
Ph.D. Thesis Committee : Grace Whang (MS&E, UCLA), Gabriel Gorelick (MS&E, UCLA), Shu Huang (MS&E, UCLA), Jiawei Tan (MS&E, UCLA), Collin Roberts (MS&E, UCLA), Sicong He (MS&E, UCLA), Kai Yang (Civil Engg., UCLA), Jiacheng Fan (MS&E, UCLA), Boya Ouyang (MS&E, UCLA), Jiangnan Wu (MS&E, UCLA), Sidi Duan (MS&E, UCLA), Xuanbing Cheng (MS&E, UCLA), Xinran Zhou (MS&E, UCLA), Zhangji Zhao (Civil Engg., UCLA)
 Shivam Sharma (Aerospace Engineering & Mechanics, University of Minnesota)
 Shashank Pathrudkar (Mechanical Engineering, Michigan Tech.).

Visitor Positions

- Institute for Mathematics and its Applications (IMA), Minneapolis, USA.
Invited participant of the “Working Group on Multiscale Strategies” at the IMA program on “Multiscale Mathematics and Computing in Science and Engineering” (June, 2018).
Travel and stay supported by the IMA.
- Hausdorff Research Institute for Mathematics, Universität Bonn, Germany.
Invited participant of the Hausdorff trimester program on “Mathematical Challenges of Materials Science and Condensed Matter Physics” (May – July, 2012).
Supported by a fellowship and travel grant from the institute.

Other Affiliations

- Member: California NanoSystems Institute (CNSI) at UCLA (2020 – present).
- Member: Center for Quantum Science and Engineering (CQSE) at UCLA (2020 – present).
- Laboratory Affiliate: Lawrence Berkeley National Laboratory, Berkeley, USA (2018 – present).

Teaching Experience

- ▷ At the University of California, Los Angeles:
 - Instructor for graduate course on *Principles of Materials Science II (MSE 201)*, Spring 2021, 2022, 2023, 2024; Fall 2024, 2025.
 - Instructor for graduate seminar course on *Exploration of Advanced Topics in Materials Science and Engineering (MSE 298)*, Spring 2021; Winter 2026 (scheduled).
 - Instructor for undergraduate laboratory course on *Computer Methods and Instrumentation in Materials Science (MSE 141L)*, Winter 2021, 2022, 2023, 2024, 2025, 2026 (scheduled).
 - Instructor for undergraduate seminar/laboratory course on *New Materials (MSE 10)*, Fall 2020, 2021, 2022, 2023, 2024, 2025.
 - Instructor for undergraduate course on *Science of Engineering Materials (MSE 104)*, Winter 2020, 2022; Fall 2022, 2023; Spring 2024, 2026 (scheduled).
- ▷ At the University of Tennessee, Knoxville:
 - Instructor for undergraduate course on *Mechanics of Materials*, Spring 2019.
 - Section instructor for undergraduate course on *Professional Topics*, Fall 2018.
 - Guest lecturer for the following course(s):
 - *Modeling and Simulation in Materials Science and Engineering* (graduate level)

Mentorship Experience

▷ At the University of Minnesota, Minneapolis:

- Teaching assistant for undergraduate course on (engineering) *Dynamics*, Fall 2007. Carried out recitations, graded tests and homework, and held office hours.
- Guest lecturer for the following course(s):
 - *Advanced Topics in Elasticity* (upper graduate level)
 - *Computational Structural Analysis* (upper undergraduate level)
 - *Aerospace Structures* (upper undergraduate level)
- Graduate students at UCLA:
 - Chenhaoyue Wang :Ph.D. student, Dept. of Materials Science and Engineering, UCLA. [Advanced to Ph.D. Candidacy]
 - Kartikey Srivastava :Ph.D. student, Dept. of Materials Science and Engineering, UCLA.
 - Zidi Yang :Ph.D. student, Dept. of Materials Science and Engineering, UCLA.
 - Hsuan Ming Yu : Ph.D. student, Dept. of Materials Science and Engineering, UCLA. **Thesis:** Nanotubes from first principle and data-driven methods: real and re-imagined. [Graduated, Currently employed at Apple Inc.]
 - Shivang Agarwal : Ph.D. student, Dept. of Electrical and Computer Engineering, UCLA. (Jointly advised with Prof. Kang Wang, Electrical Engineering, UCLA). **Thesis:** Design and applications of novel computational methods for the study of quantum properties of emergent nanomaterials and biomolecules. [Graduated, Currently employed at Sandbox AQ.]
 - Stephanie Taylor : M.S. student, Dept. of Materials Science and Engineering, UCLA. (Jointly advised with Prof. Jaime Marian). [Graduated.] **Project:** First principles and machine learning models for high entropy alloys.
 - Shihan Gao : M.S. student, Dept. of Materials Science and Engineering, UCLA. **Project:** DFT Study of Intrinsic Defects in Bulk Aluminum. [Graduated, Currently employed at Semtech Corp.]
- Undergraduate students at UCLA:
 - Maanasi Dhiraj Narayan, Dept. of Materials Science and Engineering, UCLA [Samueli Research Scholar, 2024]
 - Jennie Ren, Dept. of Materials Science and Engineering, UCLA [Samueli Research Scholar, 2023]
 - Hugo Onghai, Dept. of Materials Science and Engineering, UCLA [IBM Undergraduate Research Program Scholar] [Graduated, currently M.S. student in Cornell Tech.]
 - Alysa Phattanaphibul, Dept. of Materials Science and Engineering, UCLA (2022-2023)
 - Claire Zhang, Dept. of Mathematics, UCLA (Summer 2022)
- High school students:
 - Russell Kislik, Boaz Yoo; Science Academy, STEM Magnet (Summer 2024)
 - Philip Chen; Walnut High School (Summer 2023)
- Mentored and supervised the following students over Summer (June – August) 2017, at the Computational Research Division, Lawrence Berkeley National Laboratory:
 - Subhajit Banerjee, Graduate student (Ph.D. candidate in Civil Engineering) at the University of California, Davis; Kenneth Wu, Graduate student (M.S. in Materials Science and Engineering) at the University of California, Berkeley.