

# Amartya S. Banerjee

---

## Contact Information

Dept. of Materials Science and Engineering,  
University of California, Los Angeles.  
410 Westwood Plaza, Los Angeles, CA 90095, USA.  
Phone : (+1) 763-656-7830. Email: asbanerjee@ucla.edu  
Web (UCLA): <https://samueli.ucla.edu/people/amartya-banerjee/>  
Web (Research): <https://www.amartyabanerjee.com> • [Google Scholar Profile](#)

## 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 materials** connected to **lithium ion storage devices** and **quantum hardware**.
- **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. ([Link](#))  
Office of Equity, Diversity and Inclusion; University of California, Los Angeles.
- US Junior Oberwolfach Fellowship, 2013. ([Link](#))  
(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.

## Invited Talks

(At Workshops / Conferences / Universities / Research Labs)

- **2024:**
  - Materials Research Society (MRS) Spring Meeting (Upcoming, April, 2024), Seattle, Washington, USA.
- **2023:**
  - Advances in Computational Mechanics (ACM) conference (Upcoming, 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 *87<sup>th</sup> 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).

## Publications and Preprints

### At UCLA :

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

- Md. T. Ahmed, C. Wang, **A.S. Banerjee** and N. Admal (2023): Bicrystallography-informed Frenkel-Kontorova model for interlayer dislocations in strained 2D heterostructures (*Submitted*, [arXiv Link](#)).
- H. M. Yu, S. Sharma, O. Liebman, S. Agarwal and **A.S. Banerjee\*** (2023): Carbon Kagome Nanotubes — quasi-one-dimensional nanostructures with flat bands (*Submitted*, [arXiv Link](#)).
- S. Pathrudkar, P. Thiagarajan, S. Agarwal, **A.S. Banerjee\*** and S. Ghosh (2023): Electronic Structure Prediction of Multi-million Atom Systems Through Uncertainty Quantification Enabled Transfer Learning (*Submitted*, [arXiv Link](#)).
- 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*; 2023, 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](#) )

### Prior to UCLA :

- **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](#))

## Software

- 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](#))

## 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.

## Conference Presentations

- 58<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science, (October, 2023) Minneapolis, Minnesota, USA.
- 17<sup>th</sup> U.S. National Congress on Computational Mechanics (Upcoming, July, 2023) Albuquerque, New Mexico [2 contributed presentations].
- The 11<sup>th</sup> Annual Mach Conference (April, 2023), Baltimore, Maryland, USA.
- March Meeting of the American Physical Society (March, 2023), Las Vegas, Nevada, USA [4 contributed presentations and 1 invited presentation].
- 57<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science, College Station, Texas, USA (October, 2022). [2 contributed presentations].
- 10<sup>th</sup> International Conference on Multiscale Materials Modeling (October 2022). Baltimore, Maryland, USA.
- 19<sup>th</sup> 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].
- 16<sup>th</sup> 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 10<sup>th</sup> International Conference on Multiscale Materials Modeling, Baltimore, Maryland, USA (Scheduled for October 2020) [Cancelled due to COVID-19].
- 56<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science, St. Louis, Missouri, USA (October, 2019).
- 18<sup>th</sup> U.S. National Congress for Theoretical and Applied Mechanics, Chicago, Illinois, USA (June, 2018).
- 54<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science and ASME-AMD joint conference, Boston, Massachusetts, USA (July, 2017).
- 53<sup>rd</sup> Annual Technical Meeting of the Society of Engineering Science, College Park, Maryland, USA (October, 2016).
- 24<sup>th</sup> International Conference of Theoretical and Applied Mechanics, Montréal, Canada (August, 2016)
- 52<sup>nd</sup> Annual Technical Meeting of the Society of Engineering Science, College Station, Texas, USA (October, 2015).
- 13<sup>th</sup> U.S. National Congress on Computational Mechanics, San Diego, California (July, 2015).
- Materials Research Society – Fall 2014 Meeting & Exhibit, Boston, Massachusetts, USA (December, 2014).
- 51<sup>st</sup> Annual Technical Meeting of the Society of Engineering Science, West Lafayette, Indiana, USA (October, 2014).
- 17<sup>th</sup> U.S. National Congress on Theoretical & Applied Mechanics, East Lansing, Michigan, USA (June, 2014).
- 50<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science and ASME-AMD Annual Summer Meeting, Providence, Rhode Island, USA (July, 2013).
- 12<sup>th</sup> U.S. National Congress on Computational Mechanics, Raleigh, North Carolina (July, 2013).
- 49<sup>th</sup> Annual Technical Meeting of the Society of Engineering Science, Atlanta, Georgia, USA (October, 2012).
- 10<sup>th</sup> 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 22<sup>nd</sup> 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

- **Panelist** : National Science Foundation (NSF) proposal review panel – Mechanics of Materials & Structures Program (Engineering Directorate).
- **Grant Reviewer** : California Nanosystems Institute.
- **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) 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).
- **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](#))
- **Handling Editor** : MRS Advances (Spring 2021 MRS Meeting Edition).  
**Reviewer for the journals** : Nanoscale, ACS Nano, 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, Mathematical Reviews.
- **Committee member** for Technical Thrust Area on “Nanotechnology and Lower Scale Phenomena” for the U.S. Association for Computational Mechanics (USACM) (January 2020 – present).
- **Co-organizer of the following technical symposia:**
  - “Data-Driven and Multiscale Modeling of Energy and Quantum Materials” at the 17<sup>th</sup> U.S. National Congress on Computational Mechanics, Albuquerque, New Mexico (Upcoming, 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 15<sup>th</sup> World Congress on Computational Mechanics and 8<sup>th</sup> 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 19<sup>th</sup> 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 Rudraruaju (University of Wisconsin-Madison).
  - “Materials Modeling Across Scales: From First Principles Calculations to Mesoscale Physics” at the 16<sup>th</sup> 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 *57<sup>th</sup> 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 *56<sup>th</sup> 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 *15<sup>th</sup> 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 *54<sup>th</sup> 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 *53<sup>rd</sup> 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 *52<sup>nd</sup> 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 *13<sup>th</sup> 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 *51<sup>st</sup> 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 “Advances in the Study of Defects through Atomistic / Continuum Coupling Methods” at the *49<sup>th</sup> 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

- Samueli School of Engineering FEC Honors Committee, UCLA (2023).
- Equity, Diversity and Inclusivity Committee, Department of Materials Science & Engineering, UCLA (2022 -).
- Institute for Digital Research and Education (IDRE) Postdoctoral Fellow Selection Committee, UCLA (2021, 2022).
- Weekly departmental seminar organization, Department of Materials Science & Engineering, UCLA (Spring 2021).
- Graduate Students Admissions Committee, Department of Materials Science & Engineering, UCLA (Fall 2020, Fall 2021 and Fall 2022 applicants).
- Ph.D. Preliminary Examination Committee, Department of Materials Science & Engineering, UCLA (Winter 2021).



- Graduate Division Faculty Review Committee for the Dissertation Year Fellowship, UCLA (for 2020-2021, and 2021-2022 academic year recipients).
- Board member, Institute for Digital Research and Education (IDRE), UCLA (July 2020 - July 2023).
- Departmental representative for UCLA's DataX Initiative (Materials Science & Engineering Department).
- 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), Jianghan 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*, Spring 2021, 2022, 2023.
  - Instructor for graduate seminar course on *Exploration of Advanced Topics in Materials Science and Engineering*, Spring 2021.
  - Instructor for undergraduate laboratory course on *Computer Methods and Instrumentation in Materials Science*, Winter 2021, 2022, 2023.
  - Instructor for undergraduate seminar/laboratory course on *New Materials*, Fall 2020, 2021, 2022.
  - Instructor for undergraduate course on *Science of Engineering Materials*, Winter 2020, 2022, Fall 2022.
- ◊ 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)
- ◊ 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)

## Mentorship Experience

- Graduate students at UCLA:
  - Hsuan Ming Yu : Ph.D. student, Dept. of Materials Science and Engineering, UCLA.  
**Project:** Investigations of optical and stringly correlated properties of nanotubes using helical density functional theory.
  - Shivang Agarwal : Ph.D. student, Dept. of Electrical and Computer Engineering, UCLA. (Jointly advising with Prof. Clarice Aiello, Electrical Engineering, UCLA).  
**Project:** Ab Initio investigations of biomolecular qubits.
  - Stephanie Taylor : Ph.D. student, Dept. of Materials Science and Engineering, UCLA. (Jointly advising with Prof. Jaime Marian).
  - Chenhaoyue Wang : M.S. student (transitioning to Ph.D.), Dept. of Materials Science and Engineering, UCLA.  
**Project:** Investigations of spin transport and selectivity in 1D nanostructures.
  - Shihan Gao : M.S. student, Dept. of Materials Science and Engineering, UCLA. [Graduated, Currently employed at Semtech Corp.]
- Undergraduate students at UCLA:
  - Jennie Ren, Dept. of Materials Science and Engineering, UCLA [Samueli Summer Undergraduate Research Program]
  - Hugo Ongchai, Dept. of Materials Science and Engineering, UCLA [IBM Undergraduate Research Program Scholar]
  - Alysa Phattanaphibul, Dept. of Materials Science and Engineering, UCLA
  - Claire Zhang, Dept. of Mathematics, UCLA (Summer 2022)
- High school students:
  - 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.  
**Project:** Large scale geometry optimization calculations using Plane-Wave and Discontinuous Galerkin Density Functional Theory.
  - Kenneth Wu, Graduate student (M.S. in Materials Science and Engineering) at the University of California, Berkeley.  
**Project:** First principles relaxation studies of vacancies and dislocations in two-dimensional materials.

—