

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.
- **Usage of symmetry principles** in various areas of science and engineering, including:
 - Usage of the **Objective Structures framework** for the exploration and systematic study of unprecedented nano-materials, nano-structures and their deformations.
 - **Wave-propagation problems** in novel symmetric structures and composites.
 - **Reduction of scientific computation problems / design of computational solvers.**
- **Simulations of Energy materials** – with emphasis on, **lithium ion storage devices** and **catalytic materials** and **Quantum 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

- 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)

- **2020:**
 - Department of Mechanical Engineering, University of California, Merced;
(Upcoming: 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).

Travel Grants

From the International Union of Theoretical and Applied Mechanics (ICTAM 2016); United States Association for Computational Mechanics (USNCCM 2015, USNCCM 2013 and WCCM 2012); Institute for Mathematics and its Applications (October 2015); Materials Research Society (MRS Fall Meeting & Exhibit, 2014); Society of Engineering Science (Annual Technical Meeting, 2014); Institute for Advanced Studies/Park City Mathematics Institute (Graduate Summer School Program, 2014); International Union of Crystallography (Summer School on Mathematical Crystallography, 2010); Organizing Committee of the Workshop on Mesoscale Mechanics of Complex Materials (November, 2009).

Journal Publications

Published / Accepted :

- 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 :

- **A.S. Banerjee** (2020): Ab initio framework for systems with helical symmetry: theory, numerical implementation and applications to torsional deformations in nanostructures (Links: [arXiv](#))

In preparation :

- Shivang Agarwal and **A.S. Banerjee** (2020): On the use of helical waves for electronic structure calculations of quasi-one dimensional nanomaterials.
- Hsuan Ming Yu and **A.S. Banerjee** (2020): Symmetry adapted density functional theory calculations of the behavior of group-IV nanotubes under torsional deformations.
- **A.S. Banerjee** and R. S. Elliott (2020): A systematic framework for the study of a certain class of frequently occurring non-generic degeneracies.

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

- 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

- 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

- **Reviewer for the journals** : Nanoscale, Journal of Applied Physics, Journal of Computational Physics, Computer Physics Communications, Journal of the Mechanics and Physics of Solids, 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, Communications in Computational Physics.
- 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** :
 - “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 (Upcoming: April 2021). Co-organizers: Felipe Jornada (Stanford University), Sivan Refaely-Abramson (Weizmann Institute of Science) and Lin Lin (University of California, Berkeley).
 - “Theory and Simulation of Nanomaterials” 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 “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).
- **Helped in organizing and hosting speakers** for the Lawrence Berkeley National Lab / UC Berkeley Applied Mathematics Seminar (co-host: Prof. Lin Lin, Dept. of Mathematics).
- **Member of the following professional organizations** : 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 Students Admissions Committee, Department of Materials Science & Engineering, UCLA (for Fall 2020 applicants).
- 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 - July 2022).
- Departmental representative (for the Materials Science & Engineering Department), DataX Initiative, UCLA.
- M.S. Thesis Committee – Yushu Hu (MS&E, UCLA), Ju-Ming Tsai (MS&E, UCLA).
Ph.D. Thesis Committee – Jiacheng Fan (MS&E, UCLA), Boya Ouyang (MS&E, UCLA), Jianghan Wu (MS&E, UCLA).

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 “Multi-scale 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 undergraduate course on *Science of Engineering Materials*, Winter 2020.
- ◇ 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

- Current graduate students at UCLA:
 - Hsuan Ming Yu: Ph.D. student, Dept. of Materials Science and Engineering, UCLA.
Project: Investigations of optical and transport properties of nanotubes using helical density functional theory.
 - Olivia Liebman: Ph.D. student, Dept. of Materials Science and Engineering, UCLA. (Incoming, Fall 2020).
 - Stephanie Taylor: : Ph.D. student, Dept. of Materials Science and Engineering, UCLA. (Incoming, Fall 2020, Jointly advising with Prof. Jaime Marian).

- Shivang Agarwal: M.S. student, Dept. of Electrical and Computer Engineering, UCLA.
Project: Development of spectral methods for electronic structure calculations of quasi one dimensional nanomaterials.
- Shihan Gao: M.S. student, Dept. of Materials Science and Engineering, UCLA. [Graduated]
- 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.

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