Sanghamitra Neogi

CONTACT INFORMATION

Smead Aerospace Engineering Sciences
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EDUCATION

Ph.D., Theoretical Condensed Matter Physics, July 2011
The Pennsylvania State University, University Park, Pennsylvania USA
Dissertation Topic: "Transport in nonlinear chains and across several condensed matter interfaces"
(Advisor: Prof. Gerald D. Mahan)

M.Sc., Physics, May 2002
Indian Institute of Technology, Kanpur, India

B.Sc., Physics, December 2000
Jadavpur University, Kolkata, India

PROFESSIONAL EXPERIENCE

University of Colorado Boulder, Boulder, Colorado, USA
Department of Aerospace Engineering Sciences
Associate Professor — **August 2024 to Present**

University of Colorado Boulder, Boulder, Colorado, USA
Department of Aerospace Engineering Sciences
Assistant Professor — **August 2015 to July 2024**

Max Planck Institute for Polymer Research, Theory Group, Mainz, Germany
Postdoctoral Research Associate — **November 2011 to August 2015**

Visiting Research Scientist — **September 2015 to August 2016**

The Pennsylvania State University, University Park, Pennsylvania, USA
Graduate Teaching Assistant — **January 2003 to August 2011**

Harish-Chandra Research Institute, Allahabad, Uttar Pradesh, India
Visiting Scientist — **September 2002 to December 2002**

Indian Association for the Cultivation of Science, Kolkata, West Bengal, India
Visiting Student Fellow — **May 2001 to August 2001**

Indian Institute of Science, Bangalore, Karnataka, India
One of 20 recipient of young research fellowship — **Summer, 1997 to 2000**

HONORS, AWARDS AND FELLOWSHIPS

- Recognition from The Senate of The Colorado Legislature Convened in the First Regular Session of the Seventy-Fourth General Assembly at the State Capitol, Denver, Colorado, given on 26th Day of September, 2023
- University of Colorado Boulder Research & Innovation Office Faculty Fellow, 2024 cohort
- Mention in "The 2022 applied physics by pioneering women: a roadmap," Journal of Physics D: Applied Physics, 56(7) 073001 (2023)
- Editor's Pick, *Journal of Applied Physics*, **129**(2), 025301 (2021)
- Highly cited paper according to Web of Science (2017)

- Women in the Sciences and Engineering Institute Graduate Travel Grant Award, Pennsylvania State University, Spring 2010
- David C. Duncan Graduate Fellowship, Department of Physics, Pennsylvania State University, 2008, 2010
- Graduate Teaching Assistant Award, Department of Physics, Pennsylvania State University, 2009
- Summer School on Renormalization Group Methods for Interacting Electrons, Brasilia, Brazil, 2004 (**travel award**)
- Physics Department Braddock Fellowship, Pennsylvania State University, 2003
- Young Research Fellowship, Indian Institute of Science (IISc.), India, 1997 to 2000 (**1 of 20 recipient chosen from all-over India, 3-yrs full tuition and stipend scholarship**)
- 7^{th} rank (**1^{st} among girls**) in *10+2* level examination conducted by Government of West Bengal Council of Higher Secondary Education, India (among $\sim$ 500,000 students), 1997.
- 13^{th} rank (**1^{st} among girls**) in 10^{th} level Madhyamik Examination conducted by Government of West Bengal Board of Secondary Education, India (among $\sim$ 1 million students), 1995.

Teaching Experience

University of Colorado Boulder, Boulder, Colorado, USA
Ann And H.J. Smead Department of Aerospace Engineering Sciences

- ASEN 2001/2701-Introduction to Statics, Structures, and Materials, Fall 2016, 2017, 2021, 2022, 2023
- ASEN 4018-Senior Projects 1: Design Synthesis, Fall 2019, 2020
- ASEN 4028-Senior Projects II: Design Practicum, Spring 2020, 2021
- ASEN 5022-Dynamics of Aerospace Structures, Spring 2016, 2018, 2020, 2022, 2024
- ASEN 6519-Molecular Simulation of Materials, Spring 2017, 2019, 2021, 2023

The Pennsylvania State University, University Park, Pennsylvania USA
Department of Physics, Graduate Teaching Assistant **January 2003 to August 2011**

Refereed Journal Articles

Under Review

18. A. Pimachev and **S. Neogi**, "FluxGAN: A Physics-Aware Generative Adversarial Network Model for Generating Microstructures That Maintain Target Heat Flux." (*under review*, arxiv link)
17. A. Pimachev and **S. Neogi**, "Image to Properties: Extracting Atomic Structure Information from Band Dispersion Images of Semiconductor Heterostructures Using Machine Learning," (*under review*, arxiv link) (Patent pending)

Published

16. M. Settipalli, X. Zhang and **S. Neogi**, "Investigation of Phonon Lifetimes and Magnon-Phonon Coupling in YIG/GGG Hybrid Magnonic Systems in the Diffraction Limited Regime," *Journal of Applied Physics*, **135**(10), 104401 (2024).
Highlighted on journal front page as Editor's Pick.
15. M. Settipalli, V. S. Proshchenko and **S. Neogi**, "Effect of Electron-Phonon and Electron-Impurity Scattering on Electronic Transport Properties of Silicon/Germanium Superlattices," *Journal of Materials Chemistry C*, **10**, 7525 - 7542 (2022). (Impact Factor: 6.4)

14. A. Pimachev and **S. Neogi**, "First-Principles Prediction of Electronic Transport in Fabricated Semiconductor Heterostructures via Physics-Aware Machine Learning," *npj Computational Materials* 7, 93 (2021). (Impact Factor: 12.3) (Patent pending)

    Press Coverage: M. Hutson, "Physicists Teach AI to Simulate Atomic Clusters: Physics-informed machine learning might help verify microchips," *IEEE Spectrum*, 02 Jul 2021.

13. M. Bathe, R. Hernandez, T. Komiyama, R. Machiraju, **S. Neogi**, "Autonomous Computing Materials," *ACS Nano*, **15**(3), 3586-3592 (2021). (Impact Factor: 17.1) *All authors contributed equally to this article.*

12. V. S. Proshchenko, M. Settipalli, A. K. Pimachev, **S. Neogi**, "Role of Substrate Strain to Tune Energy Bands-Seebeck Relationship in Semiconductor Heterostructures," *Journal of Applied Physics*, **129**(2), 025301 (2021).

    Highlighted on journal front page as Editor's Pick.

11. **S. Neogi** and D. Donadio, "Anisotropic In-Plane Phonon Transport in Silicon Membranes Guided by Nanoscale Surface Resonators," *Physical Review Applied* 14, 024004 (2020). (Impact Factor: 4.985)

10. M. Settipalli and **S. Neogi**, "Theoretical Prediction of Enhanced Thermopower in n-doped Si/Ge Superlattices using Effective Mass Approximation," *Journal of Electronic Materials* **49**, 4431-4442 (2020).

9. V. S. Proshchenko, M. Settipalli, **S. Neogi**, "Optimization of Seebeck Coefficients of Strain-Symmetrized Semiconductor Heterostructures," *Applied Physics Letters*, **115**(21), 211602 (2019).

8. V. S. Proshchenko, P. P. Dholabhai, T. C. Sterling, and **S. Neogi**, "Heat and charge transport in bulk semiconductors with interstitial defects," *Physical Review B*, **99**, 014207 (2019).

7. S. Xiong, D. Selli, **S. Neogi** and D. Donadio, "Native surface oxide turns alloyed silicon membranes into nanophononic metamaterials with ultralow thermal conductivity," *Physical Review B*, **95**, 180301(R) (2017).

6. C. Mangold, **S. Neogi** and D. Donadio, "Optimal thickness of silicon membranes to achieve maximum thermoelectric efficiency: a first principles study" *Applied Physics Letters*, **109**(5), 053902 (2016).

5. S. Volz, J. Ordonez-Miranda, A. Shchepetov, M. Prunnila, J. Ahopelto, T. Pezeril, G. Vaudel, V. Gusev, P. Ruello, E. M. Weig, M. Schubert, M. Hettich, M. Grossman, T. Dekorsy, F. Alzina, B. Graczykowski, E. Chavez-Angel, J. S. Reparaz, M. R. Wagner, C. M. Sotomayor-Torres, S. Xiong, **S. Neogi** and D. Donadio, "Nanophononics: State of the Art and Perspectives" *European Physical Journal B*, **89**(1), 1-20 (2016).

    (*Highly cited paper according to Web of Science: As of January/February 2017, this highly cited paper received enough citations to place it in the top 1% of the academic field of Physics based on a highly cited threshold for the field and publication year.*)

4. **S. Neogi**, J. S. Reparaz, L. F. C. Pereira, B. Graczykowski, M. R. Wagner, M. Sledzinska, A. Shchepetov, M. Prunnila, J. Ahopelto, C. M. Sotomayor-Torres, and D. Donadio, "Tuning thermal transport in ultra-thin silicon membranes by surface nanoscale engineering" *ACS Nano*, 9 (4), pp 3820-3828 (2015). (Impact Factor: 17.1)

3. **S. Neogi** and D. Donadio, "Thermal transport in free-standing silicon membranes: Influence of dimensional reduction and surface nanostructures" *European Physical Journal B*, **88**(3), 73 (2015).

2. N. Kumar, **S. Neogi**, P. Kent, A. Bandura, J. Kubicki, D. Cole, D. Wesolowski and J. Sofo, "Hydrogen Bonds and Vibrations of Water on (110) Rutile," *Journal of Physical Chemistry C*, **113**,

13732-13740 (2009).

1. **S. Neogi** and G. D. Mahan, "Generation of traveling solitons in one-dimensional monatomic quartic lattices," *Physical Review B*, **78**(6), 064306 (2008).

Non-Peer-Reviewed Journal Articles

2. **S. Neogi** and G. D. Mahan (2016), "Lattice dynamics model calculation of Kapitza conductance at solid-fluid interfaces" (arXiv:1601.02999v1).

1. **S. Neogi** and G. D. Mahan (2009), "Pair distribution function of a square-well liquid," (arXiv:cond-mat/0909.3078v1).

In-preparation

5. **S. Neogi**, "Analytical Model of Phonon Transmission Coefficient Across one-, two- and three-dimensional Solid-Solid Interfaces."

4. Q. Moore, M. Henderson and **S. Neogi**, "Resonance Induced Phonon Localization & Guided Conduction in Silicon Membranes with Surface Nanostructures."

3. **S. Neogi**, A. Pimachev and M. Henderson, "Thermal Properties of Semiconductor Heterostructures via Physics-Informed Machine Learning."

2. A. Pimachev and **S. Neogi**, "Prediction of Atomic Contributions to Thermoelectric Coefficients of Semiconductor Heterostructures Assisted by Machine Learning."

1. A. Pimachev and **S. Neogi**, "Reinforcement Learning Model for Discovery of Multicomponent Materials."

Popular Press

3. "Revolutionizing how heat is handled in computers," *CU Boulder College of Engineering Annual Magazine*, August, 2024.

2. Olivia Doak, "CU Boulder professor lands $1 million government contract for microchip research," *Boulder Daily Camera*, August 31, 2023.

1. M. Hutson, "Physicists Teach AI to Simulate Atomic Clusters: Physics-informed machine learning might help verify microchips," *IEEE Spectrum*, 02 Jul 2021.

Patent

3. S. Neogi & A. Pimachev. 2025. Machine-Learning-Based System and Method for Determining Atomic Structure from Images of Spectral Functions. US Patent 19/043,236, filed January 31, 2025. Patent Pending.

2. S. Neogi. 2024. Systems and Methods for Thermal Modeling of Nanoscale Materials and Devices. US Patent 63/695,938, provisional application filed on 09/18/2024 , Patent pending.

1. S. Neogi & A. Pimachev. 2022. Systems and Methods to Predict Performance of Microchips and Other Electronic Devices. U.S. Patent 17/930,619, filed September 8, 2022. Patent pending.

Invited Talks

46. "Atom-to-Circuit Thermal Modeling of Microelectronic Structures Using Physics-Aware Machine Learning," NSF Panel Panel - Machine Learning for Electronics, InterPACK (International Technical Conference and Exhibition on Packaging and Integration of Electronic and Photonic Microsystems), San Jose, CA, October 8, 2024.

45. "First-Principles Prediction of Thermal Properties of Microelectronic Devices Assisted by AI," 2024 LEAD Symposium, GE Aerospace, Niskayuna, NY, October 2, 2024.

44. "Image to Properties: Extracting Information About Atomic Structures from Band Structure Images of Semiconductor Heterostructures Using AI," Novel Techniques and Applications in Electron Microscopy and Spectroscopy of Nanomaterials and their Heterostructures Symposium, 32nd International Materials Research Congress (IMRC2024), August 20, 2024.

43. "Probing Thermal Properties of Materials in Multi-Interface Microelectronic Structures Using AI," Nanoscale Heat Transport: Fundamentals and Applications Symposium, 32nd International Materials Research Congress (IMRC2024), August 20, 2024.

42. "Image to Properties—Extracting Atomic Structure Information from Spectroscopy Images using Physics-Aware AI for Design of Quantum Heterostructures," I-HUB Quantum Technology Foundation Seminar, Indian Institute of Science Education and Research, July 09, 2024.

41. "Atom to Device: Predicting Thermal and Electronic Transport Properties of Materials in Devices using Physics-Aware AI," Seminar, Department of Physics, Indian Institute of Science, Bangalore, July 08, 2024.

40. "Atom to Device: Predicting Thermal and Electronic Transport Properties of Materials in Devices using Physics-Aware AI," Seminar, Physics and Applied Mathematics Unit (PAMU), Indian Statistical Institute, Kolkata, July 05, 2024.

39. "Atomistic Thermal Model of Microelectronic Systems," Thermal Transport and Energy Conversion Symposium, 2024 MRS Spring Meeting and Exhibit, Seattle, WA, April 22-26, 2024.

38. "Atom to Device: Predicting Physical Properties of Materials in Devices using Machine Learning," "Bridging scales: At the crossroads among renormalization group, multi-scale modeling, and deep learning" workshop, European Centre for Theoretical Studies (ECT*), Trento, Italy, (Virtual) April 15-19 2024.

37. "FluxGAN: A Physics-Aware Generative Adversarial Network Model for Inverse Design of Microstructures That Maintain Target Heat Flux", "Human-machine collaboration for materials development," workshop organized by Microsystems Exploratory Council, DARPA (MTO), March 5-7, 2024, Golden, CO.

36. "From Atoms to Devices: Designing Materials for Future Devices," Intel (Virtual), February 23, 2024.

35. "AI and Thermal Management of Microelectronics," "Science of Heterogeneously Integrated Systems," workshop, Argonne National Laboratory, Lemont, IL, February 8-9, 2024.

34. "Atom to Device: Designing Materials for Resilient Devices Using First-Principles Modeling and Machine Learning Techniques," CU's Innovation in Materials Science 2023 Symposium, University of Colorado Boulder, Boulder, August 18, 2023.

33. "Theory to Experiment and Back: Machine-Learning-Assisted Pathway for Electronic Property Design," 2023 Boulder Workshop on Quantum Materials Synthesis, Boulder, July 26-29.

32. "Machine Learning Models for Electronic Properties of Complex Materials and Nanostructures," 35th Electronic Structure Workshop at University of California, Merced, 13-16 June 2023.

31. "From Atoms to Devices: AI Driven Discovery of Materials and Nanostructures," GE Research (virtual), February 17, 2023.

30. "Prediction of Electronic Properties of Nanostructured Materials: Perspective from Atomistic Modeling and Data Driven Techniques," Materials Science and Engineering seminar, University of Wyoming, November, 2022.

29. "Phonon Engineering for Quantum Memory Applications," Maybell Quantum Industries, Boulder (virtual), October, 2022.

28. "Forward and Inverse Machine Learning Assisted First-Principles Models for Designing Nanostructured Materials," Indian Institute of Technology, Gandhinagar, India, October, 2022.

27. "Investigation of Thermal Properties of Niobium Coatings Leveraging Machine Learning Approaches," Sandia ACQ Advanced Materials, (virtual) September, 2022.

26. "Phonon and Electron Transport Properties of Nanostructures: Atomistic Modeling and Data Driven Techniques," Telluride Science Research Center (TSRC) workshop on "Thermal Transport at the Nanoscale", Telluride, CO, June 21-25, 2022.

25. "Describing Phonon Properties of Nanostructures: Perspective from Atomistic Modeling and Data Driven Techniques," Materials Research Society 2022 Spring Meeting (Hybrid), Hawaii, May, 2022.

24. "Thermal Properties of Nano- & Microstructures: First-Principles Modeling and Data Driven Techniques," Thermal Protection Materials Branch, NASA Ames Research Center (virtual), April, 2022.

23. "Forward and Inverse Machine Learning Models to Assist Designing Atomic Environments of Semiconductor Heterostructures," 32nd Annual General Meeting of the Materials Research Society of India (MRSI) and Third Indian Materials Conclave, (virtual) December 20-23, 2021.

22. "Controlling Local Thermal Properties of Nanostructures: Perspective from Atomistic Modeling and Data Driven Techniques," SOPHOT: Severo Ochoa Workshop on Phononics and Thermal Transport, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Spain, (Hybrid), October 18-19, 2021.

21. "From Atoms to Devices: Bridging with First-Principles Physics and Data Driven Models," US NSF and Japanese Science and Technology Agency (JST) joint workshop on Thermal Transport, Materials Informatics and Quantum Computing, (virtual), March 22-24 2021.

20. "Controlling Vibrations at the Quantum Level: Overview and Perspective," MSE & E seminar series, University of Colorado Boulder, (virtual) October, 27, 2020.

19. "Phonon Transport in Dimensionally Confined Semiconductor Nanostructures," Virtual Brainstorming Meeting Series on Nanoscale Thermal Transport, Department of Electrical and Computer Engineering, University of British Columbia, Vancouver, Canada, August, 25, 2020.

18. "Phononic Autonomous Computing Materials," NSF-HDR-PRISM Meet & Greet Meeting, (virtual) May, 27, 2020.

17. "Deep Learning of Phonon and Electron Properties of Semiconductor Architectures," NSF-HDR Machine Learning Methods for Multi-Disciplinary Multi-Scale Problems Meet & Greet Meeting, (virtual) May, 20, 2020.

16. "Phonon and Electron Transport Properties of Defected Nanostructured Semiconductors: An Overview," Physics seminar, Indian Institute of Science, Bangalore, India, May, 2019.

15. "Phonon and Electron Transport in Defected Nanostructured Semiconductors: An Overview," Nanoscience and Technology Division, Argonne National Laboratory, August, 2018.

14. "Thermal transport at the nanoscale: How to control the quanta of heat energy?," Department of Electrical Engineering, UCLA, March, 2018.

13. "Heat Transport in Nanostructured Semiconductors: Structure-Processing-Property-Relationships," International Conference on Computational & Experimental Engineering and Sciences (ICCES), Madeira, Portugal, June 26-30, 2017.

12. "Thermal Transport at the Nanoscale: How to Control the Quanta of Energy?," Physics & Astronomy Colloquium Series, University of Wyoming, Laramie, WY, April, 2017.

11. "Thermal Transport at the Nanoscale: How to Control the Quanta of Heat Energy?," Computational Mechanics and Physics of Solids Seminar Series and Mechanical Engineering Graduate Seminar, University of Colorado, Boulder, CO, USA, October, 2016.

10. "Thermal Transport in Low-Dimensional Nanostructured Systems: Structure-Processing-Property Relationships," Mechanical and Aerospace Engineering Research Seminar, University of Colorado, Colorado Springs, CO, USA, August 2016.

9. "Thermal Transport in Low-Dimensional Nanostructured Semiconductors: Structure-Processing-Property Relationships," National Institute of Standards and Technology: Applied Chemicals and Materials Division Seminar, Boulder, CO, USA, May 2016.

8. "Structure-Processing-Property Relationships: Thermal Transport in Ultrathin Silicon Membranes," IISER (Indian Institute of Science Education and Research), Pune, India, November, 2015.

7. "Structure-Processing-vibrational Property Relationships: Toward rational design of materials with desired functionality," IBM Research, Rüschilkon, Switzerland, June, 2015.

6. "Structure-processing-vibrational property relationships: Toward rational design of materials with desired functionality," IBM T. J. Watson Research Center, Yorktown Heights, NY, USA, May, 2015.

5. "Heat transport across nanostructures and interfaces," Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, USA, December, 2014.

4. "Modeling heat transport across nanostructures and interfaces," Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY, USA, December, 2014.

3. Nanophononics Consultation Workshop (EUPHONON), (Consultation group participant), Lille, France, May, 2014.

2. "Thermal Transport Across Model Interfaces," Group seminar Theoretical Physics I, Universität Augsburg, Augsburg, Germany, February, 2014.

1. "Theoretical Investigation of Thermal Transport: Across Model Interfaces and Nanostructures," Sonderseminar des SFB 767, Universität Konstanz, Konstanz, Germany, December, 2013.

Contributed Talks Peer-reviewed abstracts

36. American Physical Society March Meeting, "FluxGAN: A Physics-Aware Generative Adversarial Network Model for Discovery of Microstructures That Maintain Target Heat Flux," Minneapolis, MN, March 3 - 8, 2024.

35. American Physical Society March Meeting, "Inverse Design of Semiconductor Heterostructures Using First-Principles Modelling and Machine Learning Approaches," Las Vegas, NV, March, 2023.

34. American Physical Society March Meeting, "Action space and features for complex multicomponent alloys and ceramics property prediction with deep reinforcement learning," Las Vegas, NV, March, 2023. (Presented by Artem Pimachev)

33. Materials Research Society Spring Meeting, "Ab Initio Modeling Data Based Autoencoder to Interpret ARPES Data and Assist Inverse Design of Semiconductor Heterostructures," (Hybrid Meeting), Hawaii, May, 2022.

32. American Physical Society March Meeting, "Accelerated materials discovery of complex multicomponent alloys and ceramics with deep reinforcement learning," (Hybrid Meeting), Chicago, IL, March, 2022. (Presented by Artem Pimachev)

31. American Physical Society March Meeting, "Machine-Learning Assisted First-Principles Model Development to Interpret ARPES Data and Assist Inverse Design of Heterostructures," (Hybrid Meeting), Chicago, IL, March, 2022.

30. Materials Research Society Spring Meeting, "Dual Crystal- and Glass-Like Heat Transport in Silicon Thin-Films with Nanscale Surface Substructures," (Virtual Meeting), April, 2021.

29. Materials Research Society Spring Meeting, "Mapping Nanoscale Thermal Transport Properties with Deep Learning Algorithms," (Virtual Meeting), April, 2021.

28. American Physical Society March Meeting, "Effect of Electron-Phonon and Electron-Ionized Impurity Interactions on Electronic Transport in Si/Ge Superlattices," (Virtual Meeting), March, 2021.

27. American Physical Society March Meeting, "First-Principles Prediction of Substrate Induced Changes in Layered Nanomaterials via Physics-Based Machine Learning," (Virtual Meeting), March, 2021.

26. American Physical Society March Meeting, "Direct and Reverse Structure-Electronic Property Relationship Prediction with Deep Learning and Bayesian Optimization," Denver, CO, USA, (Virtual Meeting), March, 2020.

25. American Physical Society March Meeting, "Strain Controlled Modulations and Anomalies in the Thermopower of Si/Ge Superlattices: A First-Principles Study," Denver, CO, USA, (Virtual Meeting), March, 2020.

24. American Physical Society March Meeting, "Phonon Localization in Ultrathin Silicon Membranes with Surface Nanostructures," Denver, CO, USA, (Virtual Meeting), March, 2020.

23. American Physical Society March Meeting, "Characterization of Phonon Dynamics and Thermal Environments in FinFET Architectures," Denver, CO, USA, (Virtual Meeting), March, 2020.

22. American Physical Society March Meeting, "Characterization of Spin-Thermal Environment Interaction Leading to Nuclear Quadrupolar Spin Relaxation," Denver, CO, USA, (Virtual Meeting), March, 2020.

21. American Physical Society March Meeting, "Optimization of Electron-Phonon Coupling and Electronic Transport in Semiconductor Superlattices," Boston, MA, USA, March, 2019.

20. American Physical Society March Meeting, "Machine Learning Electronic Transport Properties of Multilayered Semiconductor Nanostructures," Boston, MA, USA, March, 2019.

19. Materials Research Society Spring Meeting, "Heat Transport in Multicomponent Systems with Imperfect Interfaces ," Phoenix, AZ, USA, April, 2018.

18. American Physical Society March Meeting, "Heat and Electron Transport in Multi-Component Nanostructures with Imperfect Interfaces," Los Angeles, CA, USA, March, 2018.

17. American Physical Society March Meeting, "Defect induced carrier transport in semiconductor junctions," New Orleans, LA, USA, March13-17, 2017.

16. International Mechanical Engineering Congress & Exposition, "How Surface Resonators Influence Phonon Transport in Nanophononic Metamaterials," Phoenix, AZ, USA, November, 2016.

15. Materials Research Society Spring Meeting, "Spectral Analysis of Phonon Transport in Nanophononic Metamaterials," Phoenix, AZ, USA, April, 2016.

14. American Physical Society March Meeting, "Spectral Analysis of Surface Controlled Phonon Transport in Nanophononic Metamaterials," Baltimore, MD, USA, March, 2016.

13. "Mainz Materials Simulation Days 2015 - Non-Equilibrium Processes in Soft Matter", "Phononic thermal transport in ultrathin silicon membranes," Mainz, Germany, June, 2015.

12. "Phononics 2015: 3rd International Conference on Phononic Crystals/Metamaterials, Phonon Transport and Phonon Coupling", "Phononic thermal transport in nanostructured ultra-thin silicon membranes," Paris, France, June, 2015.

11. "Towards Reality in Nanoscale Materials VIII" Workshop, "To tune thermal transport in ultra-thin silicon membranes by surface nanoscale engineering," Levi, Finland, February, 2015.

10. Materials Research Society Fall Meeting, "Phononic thermal transport in nanostructured ultra-thin silicon membranes," Boston, MA, USA, December, 2014.

9. Phonons and fluctuations workshop (EUPHONON), "Phononic thermal transport in nanostructured ultra-thin silicon membranes," Le Mans, France, September, 2014.

8. Materials Research Society Spring Meeting, "Thermal Transport in Nanostructured Silicon Membranes," San Francisco, CA, USA, April, 2014.

7. DPG Spring Meeting, "Phononic Thermal Transport in Nanostructured Silicon Membranes," Dresden, Germany, April, 2014.

6. American Physical Society March Meeting, "Thermal Boundary Resistance Across Solid-Fluid Interface," Baltimore, MD, USA, March, 2013.

5. American Physical Society March Meeting, "Thermal Boundary Resistance at Ideal Gas Solid-Fluid Interfaces," Dallas, TX, USA. (**Recipient of travel grant award**). March, 2011.

4. American Physical Society March Meeting, "Kapitza Resistance at the Solid-Liquid Interface," Portland, OR, USA, March, 2010.

3. American Physical Society March Meeting, "Multiple traveling solitons in one-dimensional monatomic quartic lattices," New Orleans, LA, USA, March, 2008.

2. American Physical Society March Meeting, "Hydrogen Bonds and the Vibrational Modes of Water at Interfaces: ab-initio Molecular Dynamics meets Neutron Scattering," New Orleans, LA, USA, March, 2008.

1. American Physical Society March Meeting, "Stationary and traveling solitons in one-dimensional quartic lattices," Denver, CO, USA, March, 2007.

Posters Peer-reviewed abstracts

12. "Atomistic Thermal Model of Nanoscale Transistor," Government Microcircuit Applications & Critical Technology Conference (GOMACTech), Charleston, SC, March 18-21, 2024,

11. Quantum Control of Light and Matter Workshop, "Tuning Phonon Lifetimes and Magnon-Phonon Coupling in Hybrid Magnonic Systems for Quantum Memory Applications," Gordon Research Conference, Salve Regina University, Newport, RI, August 6 - 11, 2023.

10. CU Sandia Day, "Investigation of Thermal Properties of Porous Niobium Thermal Sprays via Image-Based Finite Element Method and Machine Learning Approaches," August 29, 2022.

9. NSF Workshop: New Frontiers in Thermal Transport, "Characterizing Phonon Dynamics in Nanostructures: Data Driven Approaches," (virtual) December 14-16 2020.

8. Materials Research Society Fall Meeting, "Statistical Learning and Prediction of Electronic Transport in Multilayered Non-Ideal Semiconductor Architectures," Boston, MA, USA, November 2018.

7. Materials Research Society Fall Meeting, "Tuning Band Structure and Electronic Transport in Multilayered Semiconductor Nanostructures," Boston, MA, USA, November 2018.

6. Crystal defects for qubits, single photon emitters and nanosensors workshop, "Characterization of Phonons in Solid-State Spin Systems," Bremen, Germany, July, 2018.

5. Materials Research Society Spring Meeting, "Surface Nanoscale Engineering to Tune Phonon Dispersion and Lifetimes in Low-Dimensional Semiconductors ," Phoenix, AZ, USA, April, 2017.

4. "Heat transfer at small scales" Workshop, "Thermal Transport Across Solid-Fluid Interfaces," Zaragoza, Spain, October, 2013.

3. "Nanophononics" Workshop, "Thermal Transport Across Solid-Fluid Interface," Bremen, Germany, August, 2013.

2. "Advanced Workshop on Energy Transport in Low-Dimensional Systems: Achievements and Mysteries" Workshop, "Thermal Boundary Resistance at Solid-Fluid Interface," Trieste, Italy, October, 2012.

1. International Symposium on Quantum Fluids and Solids, "Ground state properties of ^{4}He using a Jastrow-type product of two-atom wavefunctions as the many-body wavefunction," Northwestern University, Evanston, IL, USA, August, 2009.

*List does not include several other posters presented by student and postdoctoral advisees

INDUSTRY COLLABORATIONS

"Review on the Current Understanding of Interfacial Phonon Modes," Sponsor: Intellectual Ventures Management, LLC for the benefit of Deep Science, WA 98005, $7,500; 2019-2021. (PI: S. Neogi)

SERVICE

Internal Service

Program Faculty, Materials Science & Engineering Program. December 2020–Present
MSE Program serves as a campus-wide resource for materials research and education activities. The mission of the MSE program is to bring together faculty from across the CU campus to leverage expertise and facilities; enhance departmental materials research efforts as well as materials-related efforts that are a part of campus initiatives and programs; create a vibrant materials science research & engineering program that is both highly visible within the CU community and recognized internationally; recruit, train, and graduate outstanding doctoral students with degrees in MSE; attract outstanding faculty to the MSE Program and its participating departments; and foster the coordination of interdisciplinary materials research themes, centers and major collaborations. The MSE community is comprised of faculty affiliates from 9 departments spanning both the College of Engineering & Applied Science and the College of Arts and Sciences. Program faculty have an increased level of service connected with their affiliation. This includes teaching a MSE core or elective course regularly and/or serving on a standing MSE committee, assigned by the Director. Terms are for a period of 3 years, reviewed by a vote of the MSE Program Faculty.

Creator of Seminar Series. August 2022–Present
"CU Phonon Club, a platform to bring together CU researchers from across the campus, exploring phonon related phenomena." The club organizes monthly events where CU researchers share their research with the community and encourage discussions around the topic. The priority is given to students and postdoctoral researchers. However, the club also hosts external speakers, visitors and CU PIs, occasionally. The club is primarily run by students and postdocs with guidance from the faculty advisor.

Creator of Event Series, "Engineering Voices: Listen to CU engineers share their experiences. Share your story. Ask questions. Learn something new," in collaboration with the Broadening

Opportunities through Leadership and Diversity (BOLD) center. These events provide a platform for students, faculty, and stuff to interact, dismantling stereotypes. **2019–Present**

Recipient, Innovative Inclusion Ideas grant ($3,000) from the CU College of Engineering and Applied Science & Smead Aerospace Department of Aerospace Engineering Sciences. **2019**

Professional Service

Invited Participant, of study group discussing accelerating new materials development from ideation through commercial and/or military application, sponsored by the Microsystems Exploratory Council (MEC). The MEC is created and sponsored by DARPA's Microsystems Technology Office (MTO) to help MTO explore new research avenues and answer key questions.

Invited Member, Proposal Evaluation Board, Center for Nanoscale Materials (CNM) at Argonne National Laboratory. The CNM provides expertise and capabilities for the synthesis, fabrication, characterization, and theory of materials at the nanoscale. User access is provided through brief peer-reviewed proposals. The board members are asked to review and evaluate proposals within their area of expertise. All duties are performed virtually and do not require travel. Each year, PEB reviewers are asked to virtually attend one review cycle as a panel member. **2023-Present**

Advisor for Visioning Event organized by the NSF Engineering Research Visioning Alliance (ERVA), "Strategic Thinking for Engineering Research in the Era of Artificial Intelligence," Atlanta, GA. The executive summary and full report, *AI Engineering — A Strategic Research Framework to Benefit Society*, can be found on ERVA's website. **November 7-8, 2023**

Symposium Organization, "Frontiers in Computational Modeling of Energy Materials," 2023 American Chemical Society Rocky Mountain Regional Meeting, Laramie, WY. **September 15-17, 2023**

Symposium Organization, 2022 Materials Research Society Spring Meeting & Exhibit, "Symposium DS03: Phonon Properties of Complex Materials–Challenges in Data Generation, Data Availability and Machine Learning Approaches"; Symposium proposal was among the 71 selected through peer review process. Total 127 Symposia was proposed for the meeting. Meeting attendance: ∼10,000. **May 2022**

Mentor, American Physical Society (APS) National Mentoring Community. **2022-Present**

Session Chair, Fall 2021 International Mechanical Engineering Congress & Exposition (IMECE2021) Virtual Conference. Topic: "Modeling and simulation method." **November 1–5, 2021**

Conference Session Organization, K-9 Committee on Nanoscale Thermal Transport, ASME Heat Transfer Division, Fall 2021 International Mechanical Engineering Congress & Exposition (IMECE) virtual meeting. Topic: "Modeling and simulation method" (Co-Chair: S. Neogi). **November 1–5, 2021**

Symposium Organization, "Virtual Symposium: Harnessing Data Science for Autonomous Computing Materials." **May 27, 2021**

Panelist, US National Science Foundation (NSF) and Japanese Science and Technology Agency (JST) joint workshop on Thermal Transport, Materials Informatics and Quantum Computing. **March 22-24 2021**

Participant, NSF Workshop on New Frontiers of Thermal Transport, virtual workshop. **December 14-16, 2020 and January 4-6, 2021**

Invited Participant, Virtual Brainstorming meeting series on nanoscale thermal transport, Department of Electrical and Computer Engineering, Stewart Blusson Quantum Matter Institute, The

University of British Columbia, Vancouver, Canada. **June-August, 2020**

Invited Participant, "NSF HDR PI Meeting & Coordinating Entity Virtual Meeting." **April 28 - 30, 2020**

Invited Participant, "Microelectronics Workshop," Argonne National Laboratory, Argonne, IL. **October 15-16, 2019**

Participant, Regional Academic Collaboration (ReACt) Computational Mechanics & Sciences Workshop. **October 10-11, 2019**

Invited Member, K-9 Committee on Nanoscale Thermal Transport, within the ASME Heat Transfer Division. **2019–Present**

Invited Panelist, DOE Office of Science (DOE-SC) workshop for "Basic Research Needs for Microelectronics," Bethesda, MD, USA. **October 23-25, 2018**

Invited Participant, NSF-Harnessing the Data Revolution (HDR): Institutes for Data-Intensive Research in Science and Engineering - Ideas Labs (I-DIRSE-IL). **May 20-24, 2019**

Local Organizing Committee Member, 21st International Conference on Ternary and Multinary Compounds (ICTMC 21) Boulder, CO. **September 11-14, 2018**

Invited Member, XSEDE Resource Allocation Committee; XSEDE, the Extreme Science and Engineering Discovery Environment is supported by NSF. that allocated more than $7.3M worth of computing time to U.S. researchers in 2018. The XRAC convenes quarterly at different locations around the United States, meeting for a day and a half, starting on Sunday afternoon and finishing late Monday afternoon. "We ask the XRAC member for a three year commitment and to attend at least 3 of the 4 quarterly meetings. An XRAC member may be asked to review up to 10-15 proposals that are aligned with the area of expertise of the XRAC member." **2017-2020**

Member and Consultation Group Participant, EUPHONON project that amalgamated the activities on phonon science and technology in Europe. **2014-2015**

EDITORIAL BOARD MEMBER

Associate Editor for European Physical Journal B: Condensed Matter and Complex Systems. August 1, 2021 - December 31, 2023

PROFESSIONAL JOURNAL REFEREE

Langmuir, npj Computational Materials, Chip, Physical Review E, Journal of Applied Physics, Advanced Science, Journal of Materials Chemistry A, Physical Review Materials, Physical Review Letters, Physical Review B, Science Advances, Nature Communications, ACS Macro Letters, Journal of Physical Chemistry, Scientific Reports, Applied Physics Letters, ASME Journal of Heat Transfer, Physical Chemistry Chemical Physics

PROFESSIONAL AFFILIATIONS

American Physical Society (APS); Materials Research Society (MRS); American Society of Mechanical Engineers (ASME), Heat Transfer Division, K-9 Committee on Nanoscale Thermal Transport.