

PIERRE DARANCET

Scientist, Center for Nanoscale Materials
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EDUCATION & PROFESSIONAL PREPARATION

- Postdoctoral Research Scientist, Departments of Physics and Applied Physics, Columbia University, 2012 – 2014. *Advisors: Profs. Andrew J. Millis & Chris A. Marianetti*
- Postdoctoral Fellow, Molecular Foundry, Lawrence Berkeley National Lab, 2008 – 2012
Advisor: Prof. Jeffrey B. Neaton
- Ph.D., Université Joseph Fourier, Grenoble, France, Physics, 2008. *Advisors: Drs. Didier Mayou & Valerio Olevano*
- M.S., Université Paul Sabatier, Toulouse, France, Physics, 2005
- M.S., Institut National des Sciences Appliquées, Toulouse, France, Applied Physics, 2005

PROFESSIONAL EXPERIENCE

- 2020 – present: Scientist, Argonne National Laboratory
Principal Investigator at the Center for Nanoscale Materials, a DOE Nanoscale Science User Facility.
- 2014 - 2020: Assistant Scientist, Argonne National Laboratory
Career-track Principal Investigator at the Center for Nanoscale Materials, a DOE Nanoscale Science User Facility.
- 2016 - 2023: Fellow, Northwestern-Argonne Institute for Science and Engineering

EXPERTISE

I am a theoretical and computational condensed matter physicist. My research focuses on understanding charge, heat, and energy dynamics in materials, with a particular emphasis on quantum materials and interfaces. I develop first-principles methods for quantum and semiclassical dynamics and apply them to model contemporary scanning probes and time-resolved spectroscopy experiments.

HONORS AND AWARDS

- Ph.D. Fellowship, French Ministry of Education, Research and Technology, MENRT (2005-2008);
- Graduated with Honors (1st class), Université Paul Sabatier, Toulouse (2005),
- Impact Argonne Award for Extraordinary Effort, November 2020
- Argonne Physical Sciences & Engineering Employee of the Month, December 2020
- Argonne Physical Sciences & Engineering Employee of the Month, March 2021

- Argonne Physical Sciences & Engineering Excellence Award in the Programmatic Scientific Achievement category, September 2022
- Argonne Physical Sciences & Engineering Employee of the Month, February 2023

FUNDED PROPOSAL HISTORY

1. *Argonne National Laboratory*, Laboratory Directed Research and Development (Strategic/Prime Initiative, M3), “Managing Emission and Thermal Absorption” (**Lead PI** w/ co-PIs Maria Chan, Richard Schaller, Gary Wiederrecht, Stephen Gray, Subramanian Sankaranarayanan, Alex Martinson); FY16-FY18, total funding **\$959,780**
2. *National Science Foundation*: Northwestern University MRSEC, IRG1 “Reconfigurability in Mixed-Dimensional Heterojunctions” (lead PI: Mark Hersam, Northwestern) FY17-FY23, funding **~\$3.4M/year**
3. *Argonne National Laboratory*, Laboratory Directed Research and Development (Swift Component), “AI Robotic Platform for Solution-Processable Materials” (lead PI: Jie Xu, Argonne); FY19, total funding **\$94,841**
4. *Argonne National Laboratory*, Laboratory Directed Research and Development (Prime Initiative, Quantum Information Science) “Atomic Synthesis of Artificial Lattices for Quantum Simulation” (lead PI: Nathan Guisinger, Argonne) FY19-FY21, total funding **\$1,057,500**
5. *Argonne National Laboratory*, Laboratory Directed Research and Development (Prime Initiative, AI +Science), “AI guided metastable phase diagram of materials” (lead PI: Subramanian Sankaranarayanan, Argonne); FY19-FY21, total funding **\$400,000**
6. *Argonne National Laboratory*, Laboratory Directed Research and Development (Prime Initiative, AI +Science), “AI Robotics for Solution-Processable Materials” (**Lead PI** w/ co-PIs Jie Xu, Subramanian Sankaranarayanan, Logan Ward, Young Soo Park, Angel Yanguas-Gil); FY20, total funding **\$200,000**
7. *Argonne National Laboratory*, Laboratory Directed Research and Development (Swift) “Exploring metastable metal-nanocarbon composites for enhanced electrical and thermal conductivity” (lead PI: Subramanian Sankaranarayanan, University of Illinois at Chicago); FY21, total funding **\$25,000**
8. *Argonne National Laboratory*, Laboratory Directed Research and Development (Swift) "Transport modeling of C-in-Cu/Al nanoscale inclusions" (lead PI: Maria Chan, Argonne); FY21, total funding **\$25,000**
9. *Argonne National Laboratory*, Laboratory Directed Research and Development (Prime Initiative, AI+Science), "Inverse Microstructure Design for Enhanced Thermal and Electrical Conductivity" (Lead PI: Angel Yanguas-Gil, Argonne) FY21-FY23: total funding **\$593,480**
10. *U.S. Department of Energy*, Technology Commercialization Fund "A Machine learning toolkit for metastable phase diagram construction” (Lead PI: Subramanian Sankaranarayanan, University of Illinois at Chicago) FY21-FY23: total funding **\$250,000**
11. *U.S. Department of Energy*, Scientific User Facilities "A Digital Twin for In Silico Time-Resolved Experiments” (Lead PI: Subramanian Sankaranarayanan, University of Illinois at Chicago) FY21-FY23: total funding **\$3,600,000**
12. *U.S. Department of Energy*, Scientific User Facilities "The Atomic Quantum Information Surface Science (AQuISS) Lab” (Lead PI: Jeffrey Guest, Argonne); FY22-FY24: total funding **\$3,000,000**

13. *U.S. Department of Energy, Office of Science "Threadwork: A Transformative Co-Design Approach to Materials and Computer Architecture Research'* (Lead PI: Valerie Taylor, Argonne); FY22-FY24: total funding: **\$6,600,000**
14. *U.S. Department of Energy, Scientific User Facilities "A Digital Twin for In Silico Time-Resolved Experiments"* (Lead PI: Subramanian Sankaranarayanan, University of Illinois at Chicago) FY24-FY26: total funding **\$3,500,000**
15. *Argonne National Laboratory, Laboratory Directed Research and Development (Prime Initiative, Microelectronics), "Exascale framework for AI-enabled coupled electro-thermal modeling of 3D integrated devices."* (Lead PI w/ co-PIs Maria Chan, Subramanian Sankaranarayanan, Huihuo Zheng, Alvaro Vazquez Mayagoitia); FY24-FY25, total funding **\$400,000**

PUBLICATIONS AND PRESENTATIONS

Preprints and pending

1. **Darancet, P.** Haldar, A., Cortes, C. L., Gray, S. K., Schaller, R.D. Sharifzadeh, S. *Active Optical Elements Based on Charge Density Wave and Broken Symmetry* ANL-IN-21-069 F&L 051583-0992 Patent filed (2022).
2. Zhou, Q., Kotiuga, M., & **Darancet, P.** (2022). *Analytical Theory of Near-Field Electrostatic Effects in Two-Dimensional Materials and van der Waals Heterojunctions*. arXiv preprint *arXiv:2205.04606*.
3. Zhou, Q., Anacleto, B., Steiner, T., Kotiuga, M., & **Darancet, P.** (2021). *Engineering the Electronic Structure of Two-Dimensional Materials with Near-Field Electrostatic Effects of Self-Assembled Organic Layers*. arXiv preprint *arXiv:2109.09990*.
4. Haldar, A., Cortes, C. L., Gray, S. K., Sharifzadeh, S., & **Darancet, P.** (2021). *Giant Optomechanical Coupling in the Charge Density Wave State of Tantalum Disulfide*. arXiv preprint *arXiv:2105.08874*.

Refereed journal articles and book chapters

1. Tyner, A.C., Sur, S., Zhou, Q., Puggioni, D., **Darancet, P.**, Rondinelli, J.M., and Goswami, P., *In-plane Wilson loop for measurement of quantized non-Abelian Berry flux*. Physical Review B, 109(19), p.195149, 2024.
2. Gamage, S., Manna, S., Zajac, M., Hancock, S., Wang, Q., Singh, S., Ghafariasl, M., Yao, K., Tiwald, T.E., Park, T.J., Landau, D.P., Wen, H., Sankaranarayanan, S. K. R. S., **Darancet, P.**, Ramanathan, S., and Abate Y., *Infrared Nanoimaging of Hydrogenated Perovskite Nickelate Memristive Devices*. ACS nano, 18(3), pp.2105-2116, 2024.

3. Haldar, A., Huang, Z., Ma, X., **Darancet, P.**, and Sharifzadeh, S., *Excitation protocols for nonlinear phononics in bismuth and antimony*. *Physical Review Materials*, 8(1), p.015202 2024.
4. Jia, X., Haldar, A., Kim, J., Wang, Y., Fabbris, G., Ludwig, K., Kourtis, S., Upton, M., Liu, Y., Lu, W., Luo, X., Sun, Y.-P., Casa, D., Sharifzadeh, S., **Darancet, P.**, and Cao, Y., *Interplay of broken symmetry and delocalized excitations in the insulating state of 1T-TaS₂*. *Physical Review B*, 108(20), p.205105 2023.
5. Banik, S., Loeffler, T., Manna, S., Chan, H., Srinivasan, S., **Darancet, P.**, Hexemer, A. and Sankaranarayanan, S.K. *A Continuous Action Space Tree search for INverse desiGn (CASTING) framework for materials discovery*. *npj Computational Materials*, 9(1), p.177 2023.
6. Trainer, D.J., Srinivasan, S., Fisher, B.L., Zhang, Y., Pfeiffer, C.R., Hla, S.W., **Darancet, P.** and Guisinger, N.P. *Artificial Graphene Nanoribbons: A Test Bed for Topology and Low-Dimensional Dirac Physics*. *ACS nano* 2022.
7. Srinivasan S., Batra R., Luo D., Loeffler T., Manna S., Chan H., Yang L., Yang W., Wen J., **Darancet P.**, Sankaranarayanan, S.K.R.S. *Machine learning the metastable phase diagram of covalently bonded carbon*. *Nature Communications*. Jun 6;13(1):1-2, 2022.
8. Zhou, Q., Liu, Z. F., Marks, T. J., & **Darancet, P.** *Range-separated hybrid functionals for mixed dimensional heterojunctions: Application to phthalocyanines/MoS₂*. *APL Materials*, 9(12), 121112 2021.
9. Amsterdam, S. H., Stanev, T. K., Wang, L., Zhou, Q., Irgen-Gioro, S., Padgaonkar, S., Murthy, A.A., Sangwan, V.K., Dravid, V.P., Weiss, E.A. **Darancet, P.**, Chan, M.K.Y., Hersam, M.C., Stern, N.P. & Marks, T. J. *Mechanistic Investigation of Molybdenum Disulfide Defect Photoluminescence Quenching by Adsorbed Metallophthalocyanines*. *Journal of the American Chemical Society*, 143(41), 17153-17161, 2021.
10. Zhang, R., Clark, G., Xu, X., **Darancet, P.**, and Guest, J. R., *Observation of Single-Electron Transport and Charging on Individual Point Defects in Atomically Thin WSe₂*. *The Journal of Physical Chemistry C*, 125(25), pp.14056–14064, 2021.
11. Zhou, Q., Liu, Z.F., Marks, T.J. and **Darancet, P.**, *Electronic Structure of Metallophthalocyanines, MPc (M= Fe, Co, Ni, Cu, Zn, Mg) and Fluorinated MPc*. *The Journal of Physical Chemistry A*, 125(19), pp.4055-4061, 2021
12. Li, Q. Kolluru, V. S. C., Rahn, M. S., Schwenker, E., Li, S., Hennig, R., **Darancet, P.**, Chan M. K. Y., and Hersam, M. C., *Synthesis of borophane polymorphs through hydrogenation of borophene*. *Science* 371(6534), pp.1143-1148. 2021

13. Ryczko, K., **Darancet, P.**, and Tambllyn, I., *Inverse design of a graphene-based quantum transducer via neuroevolution*. The Journal of Physical Chemistry C, 124(48), pp.26117-26123. 2021
14. Latt, K.Z., Schlueter, J.A., **Darancet, P.**, and Hla, S.W., *Two-Dimensional Molecular Charge Density Waves in Single-Layer-Thick Islands of a Dirac Fermion System*. ACS nano, 14(7), pp.8887-8893. 2020
15. Haldar, A., Cortes, C. L., **Darancet, P.**, and Sharifzadeh, S., *Microscopic Theory of Plasmons in Substrate-supported Borophene*. Nano Letters, 20 (5), pp.2986-2992. 2020
16. Li, S., Zhong, C., Henning, A., Sangwan, V.K., Zhou, Q., Liu, X., Rahn, M.S., Wells, S.A., Park, H.Y., Luxa, J., Sofer, Z., Facchetti, A., **Darancet, P.**, Marks, T.J., Lauhon, L.J., Weiss, E.A., and Hersam, M.C., *Molecular-Scale Characterization of Photoinduced Charge Separation in Mixed-Dimensional InSe–Organic van der Waals Heterostructures*. ACS nano, 14(3), pp.3509-3518. 2020
17. Smalley, S., **Darancet, P.**, Guest, J. R., and Smerdon, J. A., *Monolayer and Bilayer Perfluoropentacene on Cu (111)*. The Journal of Physical Chemistry C, 124, 1, pp.653-658. 2020
18. Olding, J.N., Henning, A., Dong, J.T., Zhou, Q., Moody, M.J., Smeets, P.J., **Darancet, P.**, Weiss, E.A. and Lauhon, L.J., *Charge Separation in Epitaxial SnS/MoS₂ Vertical Heterojunctions Grown by Low-Temperature Pulsed MOCVD*. ACS Applied Materials & Interfaces, 11(43), pp.40543-40550. 2019
19. Zhou, Q., Cho, Y., Yang, S., Weiss, E.A., Berkelbach, T.C. and **Darancet, P.**, *Large Band Edge Tunability in Colloidal Nanoplatelets*. Nano Letters, 19(10), pp.7124-7129. 2019
20. Tung, I.C., Krishnamoorthy, A., Sadasivam, S., Zhou, H., Zhang, Q., Seyler, K.L., Clark, G., Mannebach, E.M., Nyby, C., Ernst, F., Zhu, D., Glowonia, J.M., Kozina, M.E., Song, S., Nelson, S., Kumazoe, H., Shimojo, F., Kalia, R.K., Vashista, P., **Darancet P.**, Heinz, T.F., Nakano, A., Xu, X. Lindenberg, A.M., and Wen H., *Anisotropic structural dynamics of monolayer crystals revealed by femtosecond surface x-ray scattering*. Nature Photonics, 13(6), p.425. 2019
21. Amsterdam, S.H., Stanev, T.K., Zhou, Q., Lou, A.J.T., Bergeron, H., **Darancet, P.**, Hersam, M.C., Stern, N.P. and Marks, T.J., *Electronic Coupling in Metallophthalocyanine–Transition Metal Dichalcogenide Mixed-Dimensional Heterojunctions*. ACS nano, 13(4), pp.4183-4190. 2019
22. Bishop, T.B., Farmer, E.E., Sharmin, A., Pacheco-Sanjuan, A., **Darancet, P.** and Barraza-Lopez, S., *Quantum paraelastic two-dimensional materials*. Physical Review Letters, 122(1), p.015703. 2019

23. Guo, P., Gong, J., Sadasivam, S., Xia, Y., Song, T.B., Diroll, B.T., Stoumpos, C.C., Ketterson, J.B., Kanatzidis, M.G., Chan, M.K. **Darancet, P.**, Xu, T., and Schaller, R.D. *Slow thermal equilibration in methylammonium lead iodide revealed by transient mid-infrared spectroscopy*. Nature Communications, 9(1), p.2792. 2018
24. Guo, P., Stoumpos, C.C., Mao, L., Sadasivam, S., Ketterson, J.B., **Darancet, P.**, Kanatzidis, M.G. and Schaller, R.D., *Cross-plane coherent acoustic phonons in two-dimensional organic-inorganic hybrid perovskites*. Nature Communications, 9(1), p.2019. 2018
25. Adamska, L., Sadasivam, S., Foley IV, J.J., **Darancet, P.** and Sharifzadeh, S., *First-principles investigation of borophene as a monolayer transparent conductor*. The Journal of Physical Chemistry C, 122(7), pp.4037-4045. 2018
26. Sadasivam, S., Chan, M.K. and **Darancet, P.**, *Theory of thermal relaxation of electrons in semiconductors*. Physical Review Letters, 119(13), p.136602. 2017
27. Smerdon, J.A., **Darancet, P.** and Guest, J.R., *Spatially resolved, substrate-induced rectification in C60 bilayers on copper*. The Journal of Chemical Physics, 146(9), p.092328. 2017
28. Li, H., Kim, N.T., Su, T.A., Steigerwald, M.L., Nuckolls, C., **Darancet, P.**, Leighton, J.L. and Venkataraman, L., *Mechanism for Si–Si Bond Rupture in Single Molecule Junctions*. Journal of the American Chemical Society, 138(49), pp.16159-16164. 2016
29. Diroll, B.T., Fedin, I., **Darancet, P.**, Talapin, D.V. and Schaller, R.D., *Surface-area-dependent electron transfer between isoenergetic 2D quantum wells and a molecular acceptor*. Journal of the American Chemical Society, 138(35), pp.11109-11112. 2016
30. Smerdon, J.A., Giebink, N.C., Guisinger, N.P., **Darancet, P.** and Guest, J.R., *Large spatially resolved rectification in a donor–acceptor molecular heterojunction*. Nano Letters, 16(4), pp.2603-2607. 2016
31. Kotiuga, M., **Darancet, P.**, Arroyo, C.R., Venkataraman, L. and Neaton, J.B., *Adsorption-induced solvent-based electrostatic gating of charge transport through molecular junctions*. Nano Letters, 15(7), pp.4498-4503. 2015
32. Batra, A., Meisner, J.S., **Darancet, P.**, Chen, Q., Steigerwald, M.L., Nuckolls, C. and Venkataraman, L., *Molecular diodes enabled by quantum interference*. Faraday discussions, 174, pp.79-89. 2014
33. **Darancet, P.**, Millis, A.J. and Marianetti, C.A., *Three-dimensional metallic and two-dimensional insulating behavior in octahedral tantalum dichalcogenides*. Physical Review B, 90(4), p.045134. 2014

34. Chen, Z., **Darancet, P.**, Wang, L., Crowther, A.C., Gao, Y., Dean, C.R., Taniguchi, T., Watanabe, K., Hone, J., Marianetti, C.A. and Brus, L.E., *Physical adsorption and charge transfer of molecular Br₂ on graphene*. ACS Nano, 8(3), pp.2943-2950. 2014
35. Capozzi, B., Chen, Q., **Darancet, P.**, Kotiuga, M., Buzzeo, M., Neaton, J.B., Nuckolls, C. and Venkataraman, L., *Tunable charge transport in single-molecule junctions via electrolytic gating*. Nano letters, 14(3), pp.1400-1404. 2014
36. Kim, T., **Darancet, P.**, Widawsky, J.R., Kotiuga, M., Quek, S.Y., Neaton, J.B. and Venkataraman, L., *Determination of energy level alignment and coupling strength in 4, 4'-bipyridine single-molecule junctions*. Nano Letters, 14(2), pp.794-798. 2014
37. Batra, A., **Darancet, P.**, Chen, Q., Meisner, J.S., Widawsky, J.R., Neaton, J.B., Nuckolls, C. and Venkataraman, L., *Tuning rectification in single-molecular diodes*. Nano letters, 13(12), pp.6233-6237. 2013
38. Sharifzadeh, S., **Darancet, P.**, Kronik, L. and Neaton, J.B., *Low-energy charge-transfer excitons in organic solids from first-principles: The case of pentacene*. The Journal of Physical Chemistry Letters, 4(13), pp.2197-2201. 2013
39. **Darancet, P.**, Widawsky, J.R., Choi, H.J., Venkataraman, L. and Neaton, J.B., *Quantitative current–voltage characteristics in molecular junctions from first principles*. Nano Letters, 12(12), pp.6250-6254. 2012
40. Sharifzadeh, S., Tamblyn, I., Doak, P., **Darancet, P.T.** and Neaton, J.B., *Quantitative molecular orbital energies within a G_0W_0 approximation*. The European Physical Journal B, 85(9), p.323. 2012
41. Widawsky, J.R., **Darancet, P.**, Neaton, J.B. and Venkataraman, L., *Simultaneous determination of conductance and thermopower of single molecule junctions*. Nano Letters, 12(1), pp.354-358. 2011
42. Tamblyn, I., **Darancet, P.**, Quek, S.Y., Bonev, S.A. and Neaton, J.B., *Electronic energy level alignment at metal-molecule interfaces with a G_0W_0 approach*. Physical Review B, 84(20), p.201402. 2011
43. Yee, S.K., Sun, J., **Darancet, P.**, Tilley, T.D., Majumdar, A., Neaton, J.B. and Segalman, R.A., 2011. *Inverse rectification in donor–acceptor molecular heterojunctions*. ACS nano, 5(11), pp.9256-9263. 2011
44. **Darancet, P.**, Olevano, V. and Mayou, D., *Quantum transport through resistive nanocontacts: Effective one-dimensional theory and conductance formulas for nonballistic leads*. Physical Review B, 81(15), p.155422. 2010

45. Darancet, P., Olevano, V. and Mayou, D., *Coherent electronic transport through graphene constrictions: subwavelength regime and optical analogy*. Physical Review Letters, 102(13), p.136803. 2009
46. Darancet, P., *Théorie et simulation du transport quantique dans les nanostructures* (Doctoral dissertation, Université Joseph-Fourier-Grenoble I). 2008
47. Darancet, P., Wipf, N., Berger, C., de Heer, W.A. and Mayou, D. *Quenching of the quantum Hall effect in multilayered epitaxial graphene: the role of undoped planes*. Physical Review Letters, 101(11), p.116806. 2008
48. Darancet, P., Ferretti, A., Mayou, D. and Olevano, V. *Ab initio G W electron-electron interaction effects in quantum transport*. Physical Review B, 75(7), p.075102. 2007

Invited talks at international conferences and symposia

1. MRS Spring Meeting, May 13, 2022, Honolulu, HI, United States. *Giant Optomechanical Coupling and Nonlinear Phononics in Broken-Symmetry and Charge Density Wave Materials*
2. APS March Meeting, March 15, 2021, Nashville, TN, United States (online). *Understanding electron-mediated photon-phonon interactions from first principles*
3. APS March Meeting, March 17, 2017, New Orleans, LA, United States. *Understanding Non-Equilibrium Charge Transport and Rectification at Chromophore/Metal Interfaces*
4. Telluride Science Research Center, Workshop on “Nanomaterials: Computation, Theory, and Experiment” (06/29/15-07/04/15), July 2, 2015, Telluride, CO, United States. *Understanding non-equilibrium charge transport and rectification at nanoscale interfaces*
5. The Young Engineers + Scientists Symposium 2012, March 20, 2012, Berkeley, CA, United States. *Understanding Charge Transport and Rectification at Nanoscale Interfaces*

Seminars and colloquia

1. University of Illinois at Chicago, Physics Department Seminar, March 14, 2024, Chicago, IL, United States. *Learning to shine: Control of optomechanical coupling and nonlinear phononics effects in materials*
2. University of Georgia, Physics Colloquium, November 3, 2022, Athens, GA, United States. *Understanding optomechanical coupling and nonlinear phononics effects in materials*
3. Argonne National Laboratory, NST Colloquium, September 17, 2019, Lemont, IL, United States. *Thermal Relaxation of Electrons in Semiconductors and Nanomaterials*
4. Boston University, Materials Science and Engineering, Colloquium, September 13, 2019, Boston, MA, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Two-Dimensional Materials*

5. Rutgers University, Department of Physics, April 19, 2019, Piscataway, NJ, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Two-Dimensional Materials*
6. William Paterson University of New Jersey, Department of Chemistry, April 18, 2019, Wayne, NJ, United States. *Understanding Non-Equilibrium Charge Transport and Rectification at Nanoscale Interfaces*
7. City University of New York, Graduate Research Center, April 17, 2019, New York, NY, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Two-Dimensional Materials*
8. Temple University, Department of Physics, Department, April 16, 2019, Philadelphia, PA, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Two-Dimensional Materials*
9. University of Illinois, Urbana Champaign, Materials Science and Engineering, February 7, 2018, Champaign, IL, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Nanomaterials*
10. Northwestern University, Department of Physics, January 25, 2018, Evanston, IL, United States. *Theory of Thermal Relaxation of Electrons in Semiconductors and Nanomaterials*
11. National Research Council, May 19, 2017 Ottawa, Ontario, Canada. *Theory of Thermal Relaxation of Electrons in Semiconductors*
12. University of Illinois at Chicago, Department of Physics, April 12, 2017, Chicago, IL, United States. *Understanding Non-Equilibrium Charge Transport and Rectification at Chromophore/Metal Interfaces*
13. Northwestern University, MRSEC Seminar, August 27, 2015, Evanston, IL, United States. *Understanding non-equilibrium charge transport and rectification at nanoscale interfaces*
14. Phillips 66, Research Center, August 9, 2014, Bartlesville, OK, United States. *Tailoring Nanoscale Interfaces for Energy Conversion*
15. Argonne National Laboratory, Center for Nanoscale Materials, June 25, 2014, Lemont, IL, United States. *Understanding non-equilibrium charge transport and rectification at nanoscale interfaces*
16. Oklahoma State University, Department of Physics, Stillwater, OK, United States, January 23, 2014. *Understanding Non-equilibrium Charge Transport and Rectification at Nanoscale Interfaces*
17. Rutgers University, Department of Physics, March 26, 2012, Piscataway, NJ, United States. *Understanding Non-equilibrium Charge Transport and Rectification at Nanoscale Interfaces*

18. Princeton University, Department of Chemistry, March 23, 2012, Princeton, NJ, United States. *Understanding Non-equilibrium Charge Transport and Rectification at Nanoscale Interfaces*
19. Brookhaven National Laboratory, Center for Functional Nanomaterials, February 2, 2012, Upton, NY, United States. *Understanding Non-equilibrium Charge Transport and Rectification at Nanoscale Interfaces*
20. University of Arkansas, Department of Physics, October 14, 2011, Fayetteville, AR, United States. *First-principles Studies of Out-of-Equilibrium Charge Dynamics and Rectification at Nanoscale Interfaces*
21. University of California, Berkeley, Helios Theory Seminar, April 13, 2011, Berkeley, CA, United States. *Fundamentals of Photovoltaic Effect at Nanoscale Interfaces: Absorption, Charge Separation, Out-of-equilibrium Charge Dynamics, and Rectification*
22. University of California, Berkeley, Helios Theory Seminar, May 12, 2010, Berkeley, CA, United States. *Light-induced Charge Transport in Single-Molecule Heterojunctions*
23. GDR-I Graphene-Nanotube October 19-23, 2009, Coma-Ruga, Spain. *Coherent Electronic Transport in Graphene Nanodevices: Bridging Nanoelectronics and Subwavelength Optics*
24. Institut Néel, CNRS, Séminaire Théorique, January 30, 2008, Grenoble, France. *Absence d'effet Hall quantique dans le Graphène épitaxié*

PROFESSIONAL & SYNERGISTIC ACTIVITIES

PROFESSIONAL SERVICE

- Member of Argonne Library User committee (2022-present)
- Elected Executive Member (Member at Large) of APS Prairie Section (2019-2021)
- Member of NST Colloquium committee (2016-present)
- Member of NST Space & Equipment committee (2019-present)
- Member of NST Data committee (2019-present)
- Member of Argonne LDRD Prime committee (2017)

CONFERENCE, WORKSHOP, AND SYMPOSIA ORGANIZATION

1. Sole organizer of the Center for Nanoscale Materials Theory Seminar (Hosted >100 speakers since 2019)
2. Workshop Organizer, “Artificial Intelligence for Autonomous Synthesis and Processing”. 2020 APS/CNM User meeting, April 22, 2020
3. Poster session Organizer, CNM DOE Triennial Review, June 2019
4. Workshop Organizer, “Topological Quantum Information Science: From concepts to practical realizations”. 2019 APS/CNM User meeting May 8, 2019
5. Focus Session Organizer, Electron, phonon, exciton transport in nanostructures, American Physical Society March Meeting, 2018
6. Workshop Organizer, “Heat Science and Thermal Management”, Argonne National Laboratory, June 6, 2016
7. Poster session Organizer, CNM DOE Triennial Review, June 2016
8. Focus Session Organizer: Electron, ion, exciton transport in nanostructures, American Physical Society March Meeting, 2016
9. Member of NST Colloquium committee (2016-present)

OUTREACH:

1. Judge for Argonne postdoctoral symposium 2019, 2020, 2022
2. Judge for District 58 Science Fair, 2015 - present
3. Judge for Region 9 Project Session Science Fair, 2016
4. Judge for Argonne Science Bowl, 2016.

SUPERVISION

Postdoctoral fellows:

1. Dr. Sridhar Sadasivam (Postdoctoral fellow, Argonne National Laboratory), June 2016 – January 2018
Position prior to joining the group: Graduate student, Purdue University
Position upon leaving the group: Staff Scientist position at Intel
Current position: Staff Scientist position at Intel
2. Dr. Qunfei Zhou (Postdoctoral fellow, Northwestern University); March 2018 – present
Position prior to joining the group: Postdoctoral fellow, University of Kentucky
3. Dr. Srilok Srinivasan (Postdoctoral fellow, Argonne National Laboratory, co-supervised by Dr. Subramanian Sankaranarayanan), January 2019 – April 2020
Position prior to joining the group: Graduate student, Iowa State University
Position upon leaving the group: Machine Learning Scientist at Peptilogics
Current position: Machine Learning Scientist at Peptilogics
4. Dr. Henry Chan (Postdoctoral fellow, Argonne National Laboratory, co-supervised by Dr. Subramanian Sankaranarayanan), February 2019 – September 2020
Position prior to joining the group: Postdoctoral fellow, University of Illinois at Chicago
Position upon leaving the group: Assistant Scientist, Argonne National Laboratory
Current position: Assistant Scientist, Argonne National Laboratory
5. Mr. Jack Crewse (Postdoctoral fellow, Argonne National Laboratory), August 2022 – September 2023
Position prior to joining the group: Graduate student, Missouri University of Science and Technology
Position upon leaving the group: Intellectual Property and Technology Development Manager, Polsky Center, University of Chicago
Current position: Intellectual Property and Technology Development Manager, Polsky Center, University of Chicago.

Graduate students:

6. Mr. Kevin Ryczko (Visiting Graduate Student), May – August 2018
Position prior to joining the group: Graduate student, Department of Physics, University of Ottawa
Position upon leaving the group: Graduate student, Department of Physics, University of Ottawa
Current position: Machine Learning Research Lead, SandboxAQ
7. Mr. Nicholas Rivera (Department of Energy Computational Science Graduate Fellowship Practicum), June – August 2018
Position prior to joining the group: Graduate student, Department of Physics, Massachusetts Institute of Technology

Position upon leaving the group: Graduate student, Department of Physics, Massachusetts Institute of Technology
Current position: Fellow, Harvard University.

8. Mr. Anubhab Haldar (Visiting Graduate Student), June – August 2023
Position prior to joining the group: Graduate student, Department of Electrical and Computer Engineering, Boston University
Position upon leaving the group: Staff Scientist position at Samsung
Current position: Staff Scientist position at Samsung.

Undergraduate students:

9. Mr. Praveen Balaji (Student Research Participation Program, Argonne National Laboratory), June – August 2018
Position prior to joining the group: Undergraduate student, Department of Physics and Department of Computer Science, University of Chicago
Position upon leaving the group: Undergraduate student, Department of Physics and Department of Computer Science, University of Chicago
Current position: Graduate Student, University of Illinois at Urbana Champaign
10. Mr. Trevor Steiner (Research Experience for Undergraduates, Northwestern University MRSEC, co-supervised by Dr. Qunfei Zhou), June – August 2018
Position prior to joining the group: Undergraduate student, Department of Materials Science University of Minnesota
Position upon leaving the group: Undergraduate student, Department of Materials Science University of Minnesota
Current position: Senior Layout Engineer at IonQ
11. Mr. Daniel Palmer (DOE SULI Program, Argonne National Laboratory), May – July 2020;
Position prior to joining the group: Undergraduate student, Department of Physics, University of Notre Dame
Position upon leaving the group: Research Aide, Argonne National Laboratory
Current position: Graduate Student, Department of Materials Science, University of Illinois, Urbana Champaign
12. Mr. Bukuru Anaclat (Research Experience for Undergraduates, Northwestern University MRSEC, co-supervised by Dr. Qunfei Zhou), June – August 2020
Position prior to joining the group: Undergraduate student, Department of Chemistry, Pomona College
Position upon leaving the group: Undergraduate student, Department of Chemistry, Pomona College
Current position: Graduate Student (NSF fellow), Department of Materials Science, University of Virginia

Sabbatical/visitors:

13. Professor Salvador Barraza-Lopez, May – September 2018

Position prior to joining the group: Associate Professor, Department of Physics, University of Arkansas

Position upon leaving the group: Associate Professor, Department of Physics, University of Arkansas

Current position: Associate Professor, Department of Physics, University of Arkansas

MENTORSHIP:

1. Dr. Liang Li (Argonne Postdoctoral Mentorship program), 2015 - 2019; now Data Scientist at Reonomy.
2. Dr. Matthew Sykes (Argonne Postdoctoral Mentorship program), 2015 - 2018; now Scientist at Ubiquitous Energy, Inc.
3. Dr. Peijun Guo (Argonne Postdoctoral Mentorship program), 2017 - 2019; now Assistant Professor at Yale.
4. Dr. Matthew Otten (Argonne Postdoctoral Mentorship program), 2017 – 2020; now Scientist at Hughes Research Laboratory.