

# Ravishankar Sundararaman

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## Professional appointments

- 2022–present **Priti and Mukesh Chatter '82 Career Development Chair**, Rensselaer Polytechnic Institute
- 2021–present **Associate Professor**, *Department of Materials Science and Engineering*, Rensselaer Polytechnic Institute
  - 2016–2021 **Assistant Professor**, *Department of Materials Science and Engineering*, Rensselaer Polytechnic Institute
- 2016–present **Adjunct Professor**, *Department of Physics, Applied Physics and Astronomy*, Rensselaer Polytechnic Institute
  - 2013–2016 **Postdoctoral fellow**, *Joint Center for Artificial Photosynthesis*, Lawrence Berkeley National Laboratory and California Institute of Technology

## Education

- 2013 **Ph.D. Physics**, *Cornell University*
- 2007 **B.Sc. + M.Sc. Physics**, *Indian Institute of Technology, Kanpur*

## Awards and fellowships

- 2020 Rensselaer School of Engineering Research Excellence Award
- 2020 AIME Robert Lansing Hardy Award
- 2013–2015 Materials Postdoc Fellowship, Lawrence Berkeley National Laboratory
  - 2012 Best poster at the 24<sup>th</sup> annual workshop on Electronic Structure methods
- 2007–2008 Cornell Graduate School Fellowship
  - 2007 President's Gold Medal, IIT Kanpur
  - 2002 Gold Medal at the 33<sup>rd</sup> International Physics Olympiad
- 2001 & 2002 Gold Medal at the Indian National Physics Olympiad
- 2000–2007 KVPY fellowship, Department of Science and Technology, Government of India

## Research funding

Total \$4.280M share for research group, and total \$3.317M raised as lead PI.

- 2024–2024 Discovering topological materials for BEOL interconnects using first-principles calculations and machine learning, IBM, \$100K share of \$200K collaboration as co-PI
- 2024–2024 Control of orientation and handedness of nanoscale Weyl interconnects metals on amorphous SiO<sub>2</sub>, IBM, \$100K share of \$200K collaboration as co-PI
- 2024–2024 Molecular nanoengineering of post-Cu-interconnect/low-k-dielectric interfaces for next generation nanodevice wiring, IBM, \$10K share of \$200K collaboration as co-PI

- 2023–2026 Collaborative Research: FuSe: Interconnects with Co-Designed Materials, Topology, and Wire Architecture, National Science Foundation (DMR), \$395K share of \$1.186M collaboration as co-PI
- 2023–2026 Switchable Persistent Spin Helix Devices, National Science Foundation (EPMD), \$225K share of \$450K collaboration as co-PI
- 2023–2026 Spin Entropy in Strain-Tuned Rashba Semiconductors, Air Force Office of Scientific Research, \$175K share of \$350K collaboration as co-PI
- 2022–2025 Spin-Selective Photocatalysis and Quantum Transport using Ab-Initio Density-Matrix Dynamics, Department of Energy (BES, CCS), \$582K share of \$1.2M collaboration as co-PI
- 2022–2024 EAGER: CRYO: Refrigeration across temperature scales with electrically-tunable spin-orbit materials, National Science Foundation (SSMC), \$148K share of \$297K collaboration as lead PI
- 2021–2025 Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques (BEAST), Department of Energy (BES, CCS), \$788K share of \$2.6M collaboration as lead PI
- 2020–2023 CDS&E: Ab initio ultrafast dynamics of spin, valley and charge in quantum materials, National Science Foundation (CMMT), \$231K share of \$495K collaboration as co-PI
- 2020–2022 IMPACT (Innovative Materials and Processes for Accelerated Compute Technologies), Semiconductor Research Corporation, \$390K share of \$6M center as co-PI
- 2020–2022 First-principles free energies by hybrid thermodynamic integration for phase equilibria and fission product solubility in molten salts, Department of Energy (NEUP), \$100K share of \$400K collaboration as lead PI
- 2019–2022 Van der Waals Halide Perovskite Photo-ferroelectric Synapse, National Science Foundation (EPMD), \$209K share of \$418K collaboration as co-PI
- 2019–2021 DELTA: Descriptors of Energy Landscapes by Topological Analysis, National Science Foundation (I-DIRSE-FW), \$163K share of \$1.6M collaboration as co-PI
- 2017–2021 DMREF: Collaborative Research: A Data-Centric Approach for Accelerating the Design of Future Nanostructured Polymers and Composites Systems, National Science Foundation (CMMI), \$486K share of \$791K collaboration as co-PI
- 2018–2019 Immersive experiments in the engineering classroom using Augmented Reality, RPI Teaching and Learning Collaboratory, \$10K share of \$20K collaboration as lead PI
- 2019–2019 Coupling EM waves to nanoengineered composite materials, DARPA (RadioBio, Seedling), \$100K share of \$300K collaboration as co-PI
- 2017–2018 High-performance perovskite synapse, IBM, \$68K share of \$180K collaboration as co-PI

## Open-source software contributions

- JDFTx Software for joint density-functional theory, R. Sundararaman, K. Letchworth-Weaver, D. Gunceler, K.A. Schwarz and T.A. Arias, available from <http://jdfdx.sourceforge.net>
- VASPsol Solvation module for the VASP density-functional software, K. Matthew, R. Sundararaman, K. Letchworth-Weaver, T.A. Arias and R. Hennig, available from <http://vaspsol.mse.ufl.edu>

## Invited talks

- 39. ‘First-principles materials design for nanoscale interconnects and spin transport’, University of California, Riverside, MD (November 8, 2023)
- 38. ‘First-principles materials design for nanoscale interconnects and spin transport’, National Institute of Standards and Technology, Gaithersburg, MD (September 12, 2023)

37. ‘Improving electrolyte solvation models for first-principles electrochemistry’, ACS National Meeting, San Francisco, CA (August 16, 2023)
36. ‘Density-functional approximations: from electrons to classical fluids’, and ‘Advancing solvation models from implicit to classical DFT methods’, CCMS Summer Institute Lectures, Lawrence Livermore National Laboratory (August 1, 2023)
35. ‘Improving solvation models with molecular dynamics and machine learning’, Computational Materials Chemistry workshop, Telluride (July 19, 2023)
34. ‘Directional metals for nanoscale interconnects and hot carrier extraction’, Massachusetts Institute of Technology, Boston (May 31, 2023)
33. ‘First-principles electrochemistry beyond grand-canonical density-functional theory’, 243<sup>rd</sup> ECS meeting, Boston (May 30, 2023)
32. ‘First-principles electrochemistry beyond grand-canonical density-functional theory’, Louisiana State University, Baton Rouge (Oct 7, 2022)
31. ‘*Ab initio* quantum ultrafast dynamics of electrons in materials’, MRS Spring Meeting 2022, Honolulu (May 12, 2022)
30. ‘Directional conductors for nanoscale interconnects’, Semiconductor Research Corporation Workshop, online (Feb 16, 2022)
29. ‘Towards first-principles electrochemistry with grand-canonical joint density-functional theory’, ACS National Meeting, online (August 25, 2021)
28. ‘Towards first-principles electrochemistry with grand-canonical joint density-functional theory’, University of Colorado, Boulder (April 27, 2021)
27. ‘First-principles electrochemistry with grand-canonical DFT and continuum-solvation methods’, American Physical Society March Meeting, online (March 19, 2021)
26. ‘*Ab initio* multiphysics: materials combining quantum and classical simulation techniques’, RISE Symposium, University of Puerto Rico, Cayey (Feb 1 2020)
25. ‘Leaving the collective: plasmonics from a hot electron’s point of view’, Stevens Institute of Technology, Hoboken, New Jersey (Oct 25, 2019)
24. ‘Grand-canonical continuum solvation for first-principles electrochemistry’, Computational Materials Chemistry workshop, Telluride (July 16, 2019)
23. ‘Ultrafast dynamics and transport of plasmonic hot carriers’, University of California, Santa Cruz (May 17, 2019)
22. ‘First-principles design of quantum defects in 2D materials’, American Vacuum Society Meeting, General Electric Global Research, Niskayuna, New York (May 7, 2019)
21. ‘Functional approximations for density-functional theory’, University of Colorado, Boulder (May 1, 2019)
20. ‘First-principles electrochemistry with grand-canonical DFT and continuum-solvation methods’, National Renewable Energy Laboratory, Golden (June 12, 2018)
19. ‘First-principles electrochemistry with grand-canonical DFT and continuum-solvation methods’, University of Colorado, Boulder (June 11, 2018)
18. ‘Designing nano-materials for plasmonic hot carrier applications using *ab initio* multi-physics’, CECAM Workshop on Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes, Bremen, Germany (October 12, 2017)

17. 'First-principles methods for modeling electrochemical processes', 254th ACS National Meeting, Washington DC (August 21, 2017)
16. 'Plasmonic hot carriers: Towards material design', ACS 2017 Middle Atlantic Regional Meeting, Hershey, Pennsylvania (June 5, 2017)
15. 'Material design for plasmonic and hot-carrier devices', Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 12), Waikoloa, Hawaii (May 23, 2017)
14. 'After the plasmon: designing materials to exploit non-equilibrium carriers', MRS Spring Meeting 2017, Phoenix (April 20, 2017)
13. 'Leaving the collective: plasmonics from a hot electron's point of view', International Center for Theoretical Sciences, Bengaluru, India (Dec 9, 2016)
12. 'Density-functional methods for electrochemistry and hot carrier dynamics', Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India (Dec 5, 2016)
11. 'Leaving the collective: plasmonics from a hot electron's point of view', Department of Physics, Indian Institute of Technology Delhi, New Delhi, India (Nov 30, 2016)
10. 'Density-functional methods for electrochemistry and hot carrier dynamics', Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India (Nov 28, 2016)
9. 'Leaving the collective: plasmonics from a hot electron's point of view', Tata Institute of Fundamental Research, Mumbai, India (Nov 21, 2016)
8. 'Plasmonic hot carrier dynamics: electronic structure perspectives', Workshop on physics of light-matter interactions and excited state dynamics, NG Next Basic Research Laboratory, Northrop Grumman corporation, Redondo Beach (Oct 26, 2016)
7. 'Electron interactions with liquids and light in nano-engineered energy conversion systems', Center for Nanoscale Materials, Argonne National Laboratory (Feb 24, 2016)
6. 'Electron interactions with liquids and light in nano-engineered energy conversion systems', Department of Materials Science, University of Wisconsin, Madison (Feb 22, 2016)
5. 'First principles electrochemistry using joint density functional theory and continuum solvation methods', CAMS workshop on 'Enabling Methods for Materials Innovation from Quantum to Mesoscale', University of Florida, Gainesville (June 4, 2015)
4. 'Liquids, electrochemistry and plasmonics: from electronic structure to properties at the mesoscale', Department of Materials Science and Engineering, Penn State, University Park (April 14, 2015)
3. 'Continuum solvation from joint density functional theory', Chemistry department, University of California, Riverside (Nov 10, 2014)
2. 'Nonlocal polarizable continuum models from joint density functional theory', 25<sup>th</sup> annual workshop on Electronic Structure methods, College of William and Mary, Williamsburg (June 14, 2013)
1. 'Accurate free energy functionals of liquid water for the Joint Density Functional description of solvated electronic systems', Theoretical chemistry division, Bhabha atomic research center, Mumbai, India (Aug 8, 2011)

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## Teaching experience

Fall 2018-2022 Materials Informatics and Data Science course for undergraduates & graduates

Spring 2017-2023 Advanced Electronic Properties of Materials graduate course

Spring 2021-2022 Programming for Materials Engineers undergraduate course

Summer 2020-2022 Modeling and Analysis of Uncertainty undergraduate course

Fall 2017, Spring 2020 Materials Science for Engineers undergraduate course

## Patents

3. Pending (2023), J. J. Heremans, G. Kataria, A. Gupta, M. Chandra and R. Sundararaman, 'Non-Linear Electronic Devices based on Ballistic and Hydrodynamic Electron Transport'
2. U.S. Patent No. 8987701 (2015), S. Tiwari, R. Sundararaman, S. H. Lee and M. K. Kim, 'Phase transition memories and transistors'
1. U.S. Patent No. 8080839 (2011), S. Tiwari, M. K. Kim, J. M. Rubin, S. D. Chae, C. M. Lee and R. Sundararaman, 'Electro-mechanical transistor'

## Publications

Citations: 8800+, *h*-index: 41 (Scholar)

105. *ACS Nano* **18**, 1110 (2024), Q. P. Sam, Q. Tan, C. Multunas, M. T. Kiani, R. Sundararaman, X. Ling and J. J. Cha, 'Nanomolding of Two-Dimensional Materials'
104. *Phys. Rev. Materials* **8**, L011001 (2024), A. Ghorashi, N. Rivera, B. Shi, R. Sundararaman, E. Kaxiras, J. Joannopoulos, and M. Soljacic, 'Highly confined, low-loss plasmonics based on two-dimensional solid-state defect lattices'
103. *J. Appl. Phys.* **135**, 025101 (2024), M. M. Salour, J. G. Grote, G. Kataria, M. Chandra and R. Sundararaman, 'Electromagnetic shielding using Anderson localization in nanoparticle-biopolymer composites'
102. *Phys. Rev. Lett.* **132**, 016203 (2024), M. M. Kelley, R. Sundararaman and T. A. Arias, 'Fully Ab Initio Approach to Inelastic Atom-Surface Scattering'
101. *Nature Commun.* **15**, 188 (2024), J. Xu, K. Li, U. N. Huynh, M. Fadel, J. Huang, R. Sundararaman, V. Vardeny and Y. Ping, 'How spin relaxes and dephases in bulk halide perovskites'
100. *Phys. Rev. Materials* **7**, 123801 (2023), C. Multunas, A. Grieder, J. Xu, Y. Ping and R. Sundararaman, 'Circular dichroism of crystals from first principles'
99. *J. Phys. Energy* **5**, 041501 (2023), C. Zhang, J. Cheng, Y. Chen, M. K. Y. Chan, Q. Cai, R. P. Carvalho, C. F. N. Marchiori, D. Brandell, C. M. Araujo, M. Chen, X. Ji, G. Feng, K. Goloviznina, A. Serva, M. Salanne, T. Mandai, T. Hosaka, M. Alhanash, P. Johansson, Y.-Z. Qiu, H. Xiao, M. Eikerling, R. Jinnouchi, M. M. Melander, G. Kastlunger, A. Bouzid, A. Pasquarello, S.-J. Shin, M. M. Kim, H. Kim, K. Schwarz and R. Sundararaman, '2023 Roadmap on molecular modelling of electrochemical energy materials'
98. *Chem. Mater.* **35**, 8397 (2023), S. Adhikari, J. Clary, R. Sundararaman, C. B. Musgrave, D. Vigil-Fowler and C. A. Sutton, 'Accurate Prediction of HSE06 Band Structures for a Diverse Set of Materials Using  $\Delta$ -Learning'
97. *ACS Catal.* **13**, 12894 (2023), C. R. Tezak, N. R. Singstock, A. W. Alherz, D. Vigil-Fowler, C. A. Sutton, R. Sundararaman, and C. B. Musgrave, 'Revised Nitrogen Reduction Scaling Relations from Potential-Dependent Modeling of Chemical and Electrochemical Steps'

96. *J. Chem. Phys.* **159**, 124502 (2023), T. Shah, K. Fazel, J. Lian, L. Huang, Y. Shi and R. Sundararaman, ‘First-principles molten salt phase diagrams through thermodynamic integration’
95. *ACS Energy Lett.* **8**, 4242 (2023), F. Kiani, A. R. Bowman, M. Sabzehparvar, C. O. Karaman, R. Sundararaman and G. Tagliabue, ‘Transport and Interfacial Injection of d-Band Hot Holes Control Plasmonic Chemistry’
94. *J. Appl. Phys.* **134**, 085001 (2023), J. M. Clary, M. Del Ben, R. Sundararaman and D. Vigil-Fowler, ‘Impact of solvation on the GW quasiparticle spectra of molecules’
93. *Nanomater.* **13**, 2394 (2023), P. Prabhune, Y. Comlek, A. Shandilya, R. Sundararaman, L. S. Schadler, L. C. Brinson and W. Chen, ‘Design of Polymer Nanodielectrics for Capacitive Energy Storage’
92. *Appl. Phys. Lett.* **122**, 260502 (2023), G. Ramanath, C. Rowe, G. Sharma, V. Venkataramani, J. G. Alauzun, R. Sundararaman, P. Koblinski, D. G. Sangiovanni, P. Eklund and H. Pedersen, ‘Engineering inorganic interfaces using molecular nanolayers’
91. *J. Chem. Phys.* **158**, 124122 (2023), M. Woodcox, A. Mahata, A. Hagerstrom, A. Stelson, C. Muzny, R. Sundararaman and K. Schwarz, ‘Simulating dielectric spectra: A demonstration of the direct electric field method and a new model for the nonlinear dielectric response’
90. *J. Chem. Phys.* **158**, 121102 (2023), R. Sundararaman and K. Schwarz, ‘Solvent effects determine the sign of the charges of maximum entropy and capacitance at silver electrodes’
89. *Adv. Mater.* **35**, 2208965 (2023), H. J. Han, S. Kumar, G. Jin, X. Ji, J. L. Hart, D. J. Hynek, Q. P. Sam, V. Hasse, C. Felser, D. G. Cahill, R. Sundararaman and J. J. Cha, ‘Topological Metal MoP Nanowire for Interconnect’
88. *ACS Appl. Electron. Mater.* **5**, 794 (2023), P. Gupta, E. Ruzicka, B. C. Benicewicz, R. Sundararaman and L. S. Schadler, ‘Dielectric Properties of Polymer Nanocomposite Interphases Using Electrostatic Force Microscopy and Machine Learning’
87. *J. Appl. Phys.* **133**, 045102 (2023), M. Zhang, S. Kumar, R. Sundararaman and D. Gall, ‘Resistivity scaling in CuTi determined from transport measurements and first-principles simulations’
86. *Phys. Rev. Mater.* **6**, 125201 (2022), S. Kumar, C. Multunas and R. Sundararaman, ‘Fermi surface anisotropy in plasmonic metals increases the potential for efficient hot carrier extraction’
85. *Phys. Rev. Mater.* **6**, 085002 (2022), S. Kumar, C. Multunas, B. Defay, D. Gall and R. Sundararaman, ‘Ultralow electron-surface scattering in nanoscale metals leveraging Fermi-surface anisotropy’
84. *Phys. Rev. Mater.* **6**, 083802 (2022), Y. Wang, G. Varnavides, R. Sundararaman, P. Anikeeva, J. Gooth, C. Felser and P. Narang, ‘Generalized design principles for hydrodynamic electron transport in anisotropic metals’
83. *Nat. Photonics* **16**, 529 (2022), L. Zhang, J. Jiang, C. Multunas, C. Ming, Z. Chen, Y. Hu, Z. Lu, S. Pendse, R. Jia, M. Chandra, Y. Sun, T. Lu, Y. Ping, R. Sundararaman and J. Shi, ‘Room-temperature electrically switchable spin-valley coupling in a van der Waals ferroelectric halide perovskite with persistent spin helix’
82. *Chem. Rev.* **122**, 10651 (2022), R. Sundararaman, D. Vigil-Fowler and K. Schwarz, ‘Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface’
81. *J. Appl. Phys.* **131**, 194501 (2022), A. Goudarzi, S. Behpour, R. Sundararaman, O. N. Garcia and Y. Rostovtsev, ‘Trap Dynamics of Hot Electrons in Metal-Insulator-Metal Plasmonic structures for ultra-fast optoelectronics’

80. *Phys. Rev. B* **105**, 115122 (2022), A. Habib, J. Xu, Y. Ping and R. Sundararaman, ‘Electric fields and substrates dramatically accelerate spin relaxation in graphene’
79. *J. Chem. Theory Comput.* **18**, 1286 (2022), H. M. Le, S. Kumar, N. May, E. Martinez-Baez, R. Sundararaman, B. Krishnamoorthy and A. E. Clark, ‘Behavior of Linear and Nonlinear Dimensionality Reduction for Collective Variable Identification of Small Molecule Solution-Phase Reactions’
78. *J. Chem. Phys.* **156**, 014705 (2022), A. Shandilya, K. Schwarz and R. Sundararaman, ‘Interfacial water asymmetry at ideal electrochemical interfaces’
77. *Phys. Rev. B* **104**, 184418 (2021), J. Xu, A. Habib, R. Sundararaman and Y. Ping, ‘*Ab initio* ultrafast spin dynamics in solids’
76. *Nano Lett.* **21**, 9594 (2021), J. Xu, H. Takenaka, A. Habib, R. Sundararaman and Y. Ping, ‘Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics’
75. *MRS Bulletin* **46**, 959 (2021), D. Gall, J. J. Cha, Z. Chen, H.-J. Han, C. Hinkle, J. A. Robinson, R. Sundararaman and R. Torsi, ‘Materials for interconnects’
74. *Trends Chem.* **3**, 902 (2021), S. Kumar, A. Habib and R. Sundararaman, ‘Plasmonic hot carriers scratch the surface’
73. *Phys. Rev. B* **104**, 115132 (2021), J. K. Nangoi, S. Karkare, R. Sundararaman, H. A. Padmore and T. A. Arias, ‘The importance of bulk excitations and coherent electron-photon-phonon scattering in photoemission from PbTe(111): *Ab initio* theory with experimental comparisons’
72. *J. Appl. Phys.* **130**, 034302 (2021), M. Zhang, S. Kumar, R. Sundararaman, and D. Gall, ‘Resistivity scaling in epitaxial MAX-phase  $\text{Ti}_4\text{SiC}_3(0001)$  layers’
71. *J. Appl. Phys.* **129**, 193104 (2021), J. A. Tomko, S. Kumar, R. Sundararaman, and P. E. Hopkins, ‘Temperature dependent electron-phonon coupling of Au resolved via lattice dynamics measured with sub-picosecond infrared pulses’
70. *Phys. Rev. B* **103**, 115106 (2021), N. S. Sitaraman, M. M. Kelley, R. D. Porter, M. U. Liepe, T. A. Arias, J. Carlson, A. R. Pack, M. K. Transtrum and R. Sundararaman, ‘Effect of the density of states at the Fermi level on defect free energies and superconductivity: A case study of  $\text{Nb}_3\text{Sn}$ ’
69. *Mater. Charact.* **173**, 110909 (2021), P. Gupta, L. S. Schadler and R. Sundararaman, ‘Dielectric properties of polymer nanocomposite interphases from electrostatic force microscopy using machine learning’
68. *J. Appl. Phys.* **129**, 035301 (2021), L. Chen, S. Kumar, M. Yahagi, D. Ando, Y. Sutou, D. Gall, R. Sundararaman and J. Koike, ‘Interdiffusion reliability and resistivity scaling of intermetallic compounds as advanced interconnect materials’
67. *J. Phys. Chem. A* **125**, 154 (2021), A. M. Maldonado, S. Hagiwara, T. H. Choi, F. Eckert, K. Schwarz, R. Sundararaman, M. Otani and J. A. Keith, ‘Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms’
66. *J. Phys. Chem. Lett.* **12**, 440 (2021), K. Schwarz, M. C. Groenenboom, T. P. Moffat, R. Sundararaman and J. Vinson, ‘Resolving the Geometry/Charge Puzzle of the  $c(2 \times 2)$ -Cl Cu(100) Electrode’
65. *J. Phys. Chem. B* **124**, 7717 (2020), A. Habib, H. Vijayamohanan, C. K. Ullal and R. Sundararaman, ‘Coupled Electromagnetic and Reaction Kinetics Simulation of Super-Resolution Interference Lithography’

64. *Nat. Mater.* **19**, 1312 (2020), G. Tagliabue, J. S. DuChene, M. Abdellah, A. Habib, D. J. Gosztola, Y. Hattori, W.-H. Cheng, K. Zheng, S. E. Canton, R. Sundararaman, J. Sa and H. A. Atwater, ‘Ultrafast hot-hole injection modifies hot-electron dynamics in Au/p-GaN heterostructures’
63. *Phys. Rev. Mater.* **4**, 074011 (2020), R. Sundararaman, T. Christensen, Y. Ping, N. Rivera, J. D. Joannopoulos, M. Soljacic and P. Narang, ‘Plasmonics in argentene’
62. *Nat. Commun.* **11**, 2780 (2020), J. Xu, A. Habib, S. Kumar, F. Wu, R. Sundararaman and Y. Ping, ‘Spin-phonon relaxation from a universal *ab initio* density-matrix approach’
61. *Surf. Sci. Rep.* **75**, 100492 (2020), K. Schwarz and R. Sundararaman, ‘The electrochemical interface in first-principles calculations’
60. *J. Phys. D: Appl. Phys.* **53**, 333001 (2020), L. S. Schadler, L. C. Brinson, W. Chen, R. Sundararaman, P. Gupta, P. Prabhune, A. Iyer, Y. Wang and A. Shandilya, ‘A perspective on the data-driven design of polymer nanodielectrics’
59. *ACS Nano* **14**, 5788 (2020), G. Tagliabue, J. S. DuChene, A. Habib, R. Sundararaman and H. A. Atwater, ‘Hot Hole versus Hot Electron Transport at Copper/GaN Heterojunction Interfaces’
58. *Sci. Adv.* **6**, eaay4213 (2020), Y. Hu, F. Florio, Z. Chen, W. A. Phelan, M. A. Siegler, Z. Zhou, Y. Guo, R. Hawks, J. Jiang, J. Feng, L. Zhang, B. Wang, Y. Wang, D. Gall, E. F. Palermo, Z. Lu, X. Sun, T.-M. Lu, H. Zhou, Y. Ren, E. Wertz, R. Sundararaman and J. Shi, ‘A chiral switchable photovoltaic ferroelectric 1D perovskite’
57. *Phys. Rev. B* **101**, 054103 (2020), D. Wang and R. Sundararaman, ‘Layer dependence of defect charge transition levels in two-dimensional materials’
56. *J. Mater. Research* **35**, 931 (2020), A. Shandilya, L. S. Schadler and R. Sundararaman, ‘First-principles identification of localized trap states in polymer nanocomposite interfaces’
55. *Soft Matter* **15**, 9336 (2019), A. A. Karanastasis, G. S. Kenath, R. Sundararaman and C. K. Ullal, ‘Quantification of functional crosslinker reaction kinetics via super-resolution microscopy of swollen microgels’
54. *Phys. Rev. Mater.* **3**, 083803 (2019), D. Wang and R. Sundararaman, ‘Substrate effects on charged defects in two-dimensional materials’
53. *J. Phys. Chem. C* **123**, 21120 (2019), S. Kassavetis, B. D. Ozsdolay, N. Kalfagiannis, A. Habib, J.-H. Tortai, S. Kerdsonpanya, R. Sundararaman, M. Stchakovsky, D. V. Bellas, D. Gall and P. Patsalas, ‘Near-Zero Negative Real Permittivity in Far Ultraviolet: Extending Plasmonics and Photonics with B1-MoNx’
52. *Phys. Rev. Mater.* **3**, 075201 (2019), A. S. Jermyn, G. Tagliabue, H. A. Atwater, W. A. Goddard III, P. Narang and R. Sundararaman, ‘Transport of hot carriers in plasmonic nanostructures’
51. *Phys. Rev. B* **99**, 165409 (2019), M. Chandra, G. Kataria, D. Sahdev and R. Sundararaman, ‘Hydrodynamic and ballistic AC transport in two-dimensional Fermi liquids’
50. *Nano Lett.* **19**, 3091 (2019), M.-N. Su, C. Ciccarino, S. Kumar, P. Dongare, S. A. H. Jebeli, D. Renard, Y. Zhang, B. Ostovar, W.-S. Chang, P. Nordlander, N. J. Halas, R. Sundararaman, P. Narang, and S. Link, ‘Ultrafast Electron Dynamics in Single Aluminum Nanostructures’
49. *Am. J. Phys.* **87**, 291 (2019), C. K. Ullal, J. Shi and R. Sundararaman, ‘Electron mobility in graphene without invoking the Dirac equation’



48. *Phys. Rev. B* **99**, 075430 (2019), M. E. Trusheim, N. H. Wan, K. C. Chen, C. J. Ciccarino, J. Flick, R. Sundararaman, G. Malladi, E. Bersin, M. Walsh, B. Lienhard, H. Bakhru, P. Narang, and D. Englund, ‘Lead-related quantum emitters in diamond’
47. *Phys. Rev. B* **98**, 115130 (2018), J. Coulter, R. Sundararaman and P. Narang, ‘Microscopic origins of hydrodynamic transport in the type-II Weyl semimetal WP<sub>2</sub>’
46. *Nat. Commun.* **9**, 3394 (2018), G. Tagliabue, A. S. Jermyn, R. Sundararaman, A. J. Welch, J. S. DuChene, R. Pala, A. R. Davoyan, P. Narang and H. A. Atwater, ‘Quantifying the role of surface plasmon excitation and hot carrier transport in plasmonic devices’
45. *Nano Lett.* **18**, 5709 (2018), C. J. Ciccarino, T. Christensen, R. Sundararaman and P. Narang, ‘Dynamics and Spin-Valley Locking Effects in Monolayer Transition Metal Dichalcogenides’
44. *Electrochim. Acta* **281**, 127 (2018), M. C. Figueiredo, D. Hiltrop, R. Sundararaman, K. A. Schwarz and M. T. M. Koper, ‘Absence of diffuse double layer effect on the vibrational properties and oxidation of chemisorbed carbon monoxide on a Pt(111) electrode’
43. *J. Opt.* **20**, 064001 (2018), A. Habib, F. Florio and R. Sundararaman, ‘Hot carrier dynamics in plasmonic transition metal nitrides’
42. *J. Appl. Phys.* **123**, 155107 (2018), T. Zhou, P. Zheng, S. C. Pandey, R. Sundararaman and D. Gall, ‘The electrical resistivity of rough thin films: A model based on electron reflection at discrete step edges’
41. *J. Chem. Phys.* **148**, 144105 (2018), R. Sundararaman, K. Letchworth Weaver and K. A. Schwarz, ‘Improving Accuracy of Electrochemical Capacitance and Solvation Energetics in First-Principles Calculations’
40. *IEEE Trans. Magn.* **54**, 1 (2018), F. Florio, G. Sinha and R. Sundararaman, ‘Designing High-Accuracy Permanent Magnets for Low-Power Magnetic Resonance Imaging’
39. *ACS Photonics* **5**, 384 (2018), G. T. Papadakis, P. Narang, R. Sundararaman, N. Rivera, H. Buljan, N. Engheta and M. Soljacic, ‘Ultra-light Å-scale Optimal Optical Reflectors’
38. *Phys. Rev. Mater.* **1**, 071001(R) (2017), F. Wu, A. Galatas, R. Sundararaman, D. Rocca and Y. Ping, ‘First-principles engineering of charged defects for two-dimensional quantum technologies’
37. *Nat. Commun.* **8**, 1656 (2017), O. Lozan, R. Sundararaman, B. Ea-Kim, J.-M. Rampnoux, P. Narang, S. Dilhaire and P. Lalanne, ‘Increased rise time of electron temperature during adiabatic plasmon focusing’
36. *SoftwareX* **6**, 278 (2017), R. Sundararaman, K. Letchworth-Weaver, K. A. Schwarz, D. Gunceler, Y. Ozhabes and T.A. Arias, ‘JDFTx: software for joint density-functional theory’
35. *Nat. Commun.* **8**, 998 (2017), B. de Nijs, F. Benz, S. J. Barrow, D. O. Sigle, R. Chikkaraddy, A. Palma, C. Carnegie, M. Kamp, R. Sundararaman, P. Narang, O. A. Scherman and J. J. Baumberg, ‘Plasmonic tunnel junctions for single-molecule redox chemistry’
34. *J. Phys. Chem. Lett.* **8**, 5344 (2017), R. Sundararaman, M. C. Figueiredo, M. T. M. Koper and K. A. Schwarz, ‘Electrochemical Capacitance of CO-terminated Pt(111) is Dominated by CO-Solvent Gap’
33. *RSC Advances* **7**, 43660 (2017), L. Blumenthal, J. M. Kahk, R. Sundararaman, P. Tangney and J. Lischner, ‘Energy level alignment at semiconductor-water interfaces from atomistic and continuum solvation models’
32. *Angew. Chem. Int. Ed.* **56**, 13070 (2017), S. Choudhury, Z. Tu, S. Stalin, D. Vu, K. Fawole, D. Gunceler, R. Sundararaman and L. Archer, ‘Electroless Formation of Hybrid Lithium Anodes for Fast Interfacial Ion Transport’

31. *Nat. Commun.* **8**, 14880 (2017), E. Cortes, W. Xie, J. Cambiasso, A. Jermyn, R. Sundararaman, P. Narang, S. Schlucker and S. A. Maier, ‘Plasmonic hot electron transport drives nano-localized chemistry’
30. *Adv. Opt. Mater.* **5**, 1600914 (2017), P. Narang, L. Zhao, S. Claybrook and R. Sundararaman, ‘Effects of Interlayer Coupling on Hot Carrier Dynamics in Graphene-Derived van der Waals Heterostructures’
29. *J. Chem. Phys.* **146**, 114104 (2017), R. Sundararaman, W. A. Goddard III and T. A. Arias, ‘Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry’
28. *J. Chem. Phys.* **146**, 104109 (2017), R. Sundararaman and Y. Ping, ‘First-principles electrostatic potentials for reliable alignment at interfaces and defects’
27. *J. Chem. Phys.* **146**, 084111 (2017), R. Sundararaman and K. Schwarz, ‘Evaluating continuum solvation models for the electrode-electrolyte interface: Challenges and strategies for improvement’
26. *Phys. Rev. Lett.* **118**, 087401 (2017), A. Brown, R. Sundararaman, P. Narang, A. M. Schwartzberg, W.A. Goddard III and H.A. Atwater, ‘Experimental and *Ab initio* Ultrafast Carrier Dynamics in Plasmonic Nanoparticles’
25. *Phys. Rev. B* **94**, 075120 (2016), A. Brown, R. Sundararaman, P. Narang, W.A. Goddard III and H.A. Atwater, ‘*Ab initio* phonon coupling and optical response of hot electrons in plasmonic metals’
24. *J. Phys. Chem. C* **120**, 21056 (2016), P. Narang, R. Sundararaman, A. Jermyn, W.A. Goddard III and H.A. Atwater, ‘Cubic Nonlinearity Driven Up-Conversion in High-Field Plasmonic Hot Carrier Systems’
23. *Phys. Chem. Chem. Phys.* **18**, 16216 (2016), K. Schwarz, B. Xu, Y. Yan and R. Sundararaman, ‘Partial oxidation of step-bound water leads to anomalous pH effects on metal electrode step-edges’
22. *Nanophotonics* **5**, 96 (2016), P. Narang, R. Sundararaman and H.A. Atwater, ‘Plasmonic hot carrier dynamics in solid-state and chemical systems for energy conversion’
21. *J. Am. Chem. Soc.* **138**, 483 (2016), H. Xiao, T. Cheng, W.A. Goddard III and R. Sundararaman, ‘Mechanistic Explanation of the pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu (111)’
20. *ACS Nano* **10**, 957 (2016), A. Brown, R. Sundararaman, P. Narang, W.A. Goddard III and H.A. Atwater, ‘Non-Radiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces and Geometry’
19. *Phys. Chem. Chem. Phys.* **17**, 30499 (2015), Y. Ping, R. Sundararaman and W.A. Goddard III, ‘Solvation effects on the band edge positions of photocatalysts from first principles’
18. *Phys. Chem. Chem. Phys.* **17**, 20805 (2015), K.A. Schwarz, R. Sundararaman, T.P. Moffat and T. Allison, ‘Formic acid oxidation on platinum: a simple mechanistic study’
17. *J. Chem. Phys.* **142**, 214101 (2015), K.A. Schwarz, R. Sundararaman and T.A. Arias, ‘Computationally efficient dielectric calculations of molecular crystals’
16. *J. Chem. Phys.* **142**, 064107 (2015), R. Sundararaman and W.A. Goddard III, ‘The charge-asymmetric nonlocally-determined local-electric (CANDLE) solvation model’
15. *J. Chem. Phys.* **142**, 054102 (2015), R. Sundararaman, K.A. Schwarz, K. Letchworth-Weaver and T.A. Arias, ‘Spicing up continuum solvation models with SaLSA: The spherically-averaged liquid susceptibility *ansatz*’

14. *Nat. Commun.* **5**, 5788 (2014), R. Sundararaman, P. Narang, A. Jermyn, W.A. Goddard III and H.A. Atwater, 'Theoretical predictions for hot-carrier generation from surface plasmon decay'
13. *J. Chem. Phys.* **141**, 134105 (2014), R. Sundararaman, D. Gunceler and T.A. Arias, 'Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models'
12. *J. Chem. Phys.* **140**, 144504 (2014), R. Sundararaman, K. Letchworth-Weaver and T.A. Arias, 'A recipe for free-energy functionals of polarizable molecular fluids'
11. *Nano Lett.* **14**, 1453 (2014), M.E. Holtz, Y. Yu, D. Gunceler, J. Gao, R. Sundararaman, K.A Schwarz, T.A. Arias, H.D. Abruna and D.A. Muller, 'Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of Battery Electrode and Electrolyte'
10. *J. Chem. Phys.* **140**, 084106 (2014), K. Matthew, R. Sundararaman, K. Letchworth-Weaver, T.A. Arias and R. Hennig, 'Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways'
9. *Comp. Phys. Comm.* **185**, 818 (2014), R. Sundararaman and T.A. Arias, 'Efficient classical density-functional theories of rigid-molecular fluids and a simplified free energy functional for liquid water'
8. *Phys. Rev. B* **87**, 165122 (2013), R. Sundararaman and T.A. Arias, 'Ideal regularization of the Coulomb singularity in exact exchange by Wigner-Seitz truncated interactions: towards chemical accuracy in non-trivial systems'
7. *Mod. Sim. Mat. Sci. Eng.* **21**, 074005 (2013), D. Gunceler, K. Letchworth-Weaver, R. Sundararaman, K.A. Schwarz and T.A. Arias, 'The importance of nonlinear fluid response in joint density-functional theory studies of battery systems'
6. *J. Chem. Phys.* **137**, 044107 (2012), R. Sundararaman, K. Letchworth-Weaver and T.A. Arias, 'A computationally efficacious free-energy functional for studies of inhomogeneous liquid water'
5. *Phys. Rev. B* **85**, 201102(R) (2012), K.A. Schwarz, R. Sundararaman, K. Letchworth-Weaver, T.A. Arias and R.G. Hennig, 'Framework for solvation in quantum Monte Carlo'
4. *J. Nanosci. and Nanotech.* **12**, 423 (2012), M. Kim, R. Sundararaman, S. Tiwari and J.-W. Lee, 'Charge Trapping Devices Using a Bilayer Oxide Structure'
3. *IEEE Electron Device Letters* **32**, 414 (2011), J.M. Rubin, R. Sundararaman, M. Kim and S. Tiwari, 'A Low-voltage Torsion Nanorelay'
2. *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, 'A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices'
1. *IEEE Trans. Magn.*, **44**, 2351 (2008), G. Sinha, R. Sundararaman, and G. Singh, 'Design Concepts of Optimized MRI Magnet'