

## List of publications: Ravishankar Sundararaman

110. *npj Comput. Mater.* **10**, 84 (2024), S. Kumar, Y.-H. Tu, S. Luo, N. A. Lanzillo, T.-R. Chang, G. Liang, R. Sundararaman, H. Lin and C.-T. Chen, ‘Surface-dominated conductance scaling in Weyl semimetal NbAs’
109. *J. Comput. Chem.* , in press (2024), K. Fazel, N. Karimitari, T. Shah, C. Sutton and R. Sundararaman, ‘Improving the reliability of machine learned potentials for modeling inhomogeneous liquids’
108. *J. Appl. Phys.* **135**, 160401 (2024), A. Stelson, D. Laage, K. Schwarz and R. Sundararaman, ‘Solid-liquid interfaces: Atomic-scale structure and dynamics’
107. *Light: Sci. Appl.* **13**, 91 (2024), A. R. Bowman, A. R. Echarri, F. Kiani, F. Iyikanat, T. V. Tsoulos, J. D. Cox, R. Sundararaman, F. J. García de Abajo and G. Tagliabue, ‘Quantum-mechanical effects in photoluminescence from thin crystalline gold films’
106. *Curr. Opin. Solid State Mater. Sci.* **29**, 101145 (2024), Z. Wang, Z. Chen, R. Xu, H. Zhu, R. Sundararaman and J. Shi, ‘Challenges and opportunities in searching for Rashba-Dresselhaus materials for efficient spin-charge interconversion at room temperature’
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’
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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’

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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’
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78. *J. Chem. Phys.* **156**, 014705 (2022), A. Shandilya, K. Schwarz and R. Sundararaman, ‘Interfacial water asymmetry at ideal electrochemical interfaces’
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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’
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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’
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