

List of publications: Ravishankar Sundararaman

1. *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_2 ’
2. *Nature 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’
3. *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’
4. *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’
5. *J. Opt.* **20**, 064001 (2018), A. Habib, F. Florio and R. Sundararaman, ‘Hot carrier dynamics in plasmonic transition metal nitrides’
6. *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’
7. *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’
8. *IEEE Trans. Magn.* **54**, 1 (2018), F. Florio, G. Sinha and R. Sundararaman, ‘Designing High-Accuracy Permanent Magnets for Low-Power Magnetic Resonance Imaging’
9. *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’
10. *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’
11. *Nature 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’
12. *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’
13. *Nature 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’
14. *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’
15. *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’
16. *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’
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19. *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’
20. *J. Chem. Phys.* **146**, 104109 (2017), R. Sundararaman and Y. Ping, ‘First-principles electrostatic potentials for reliable alignment at interfaces and defects’
21. *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’
22. *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’
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27. *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)’
28. *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’
29. *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’
30. *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’
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37. *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’
38. *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’

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40. *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’
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45. *IEEE Electron Device Letters* **32**, 414 (2011), J.M. Rubin, R. Sundararaman, M. Kim and S. Tiwari, ‘A Low-voltage Torsion Nanorelay’
46. *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, ‘A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices’
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