

List of publications: Ravishankar Sundararaman

1. *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’
2. *J. Opt.* **20**, 064001 (2018), A. Habib, F. Florio and R. Sundararaman, ‘Hot carrier dynamics in plasmonic transition metal nitrides’
3. *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’
4. *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’
5. *IEEE Trans. Magn.* **54**, 1 (2018), F. Florio, G. Sinha and R. Sundararaman, ‘Designing High-Accuracy Permanent Magnets for Low-Power Magnetic Resonance Imaging’
6. *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’
7. *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’
8. *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’
9. *SoftwareX* **6**, 278 (2017), R. Sundararaman, K. Letchworth-Weaver, K. A. Schwarz, D. Gunceler, Y. Ozhables and T.A. Arias, ‘JDFTx: software for joint density-functional theory’
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11. *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’
12. *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’
13. *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’
14. *Nature 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’
15. *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’
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17. *J. Chem. Phys.* **146**, 104109 (2017), R. Sundararaman and Y. Ping, ‘First-principles electrostatic potentials for reliable alignment at interfaces and defects’

18. *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’
19. *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’
20. *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’
21. *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’
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28. *J. Chem. Phys.* **142**, 214101 (2015), K.A. Schwarz, R. Sundararaman and T.A. Arias, ‘Computationally efficient dielectric calculations of molecular crystals’
29. *J. Chem. Phys.* **142**, 064107 (2015), R. Sundararaman and W.A. Goddard III, ‘The charge-asymmetric nonlocally-determined local-electric (CANDLE) solvation model’
30. *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*’
31. *Nature 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’
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37. *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’

38. *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’
39. *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’
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42. *IEEE Electron Device Letters* **32**, 414 (2011), J.M. Rubin, R. Sundararaman, M. Kim and S. Tiwari, ‘A Low-voltage Torsion Nanorelay’
43. *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, ‘A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices’
44. *IEEE Trans. Magn.*, **44**, 2351 (2008), G. Sinha, R. Sundararaman, and G. Singh, ‘Design Concepts of Optimized MRI Magnet’