

List of publications: Ravishankar Sundararaman

1. *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’
2. *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’
3. *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’
4. *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’
5. *ACS Photonics*, accepted (2017), G. T. Papadakis, P. Narang, R. Sundararaman, N. Rivera, H. Buljan, N. Engheta and M. Soljacic, ‘Ultra-light Å-scale Optimal Optical Reflectors’
6. *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’
7. *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’
8. *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’
9. *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’
10. *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’
11. *J. Chem. Phys.* **146**, 104109 (2017), R. Sundararaman and Y. Ping, ‘First-principles electrostatic potentials for reliable alignment at interfaces and defects’
12. *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’
13. *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’
14. *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’
15. *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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17. *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’

18. *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)’
19. *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’
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21. *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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23. *J. Chem. Phys.* **142**, 064107 (2015), R. Sundararaman and W.A. Goddard III, ‘The charge-asymmetric nonlocally-determined local-electric (CANDLE) solvation model’
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27. *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’
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29. *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’
30. *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’
31. *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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37. *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, ‘A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices’
38. *IEEE Transactions on Magnetism*, **44**, 2351 (2008), G. Sinha, R. Sundararaman, and G. Singh, ‘Design Concepts of Optimized MRI Magnet’