

## List of publications: Ravishankar Sundararaman

1. *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’
2. *Angewandte Chemie*, DOI: 10.1002/anie.201707754 (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’
3. *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’
4. *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’
5. *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’
6. *J. Chem. Phys.* **146**, 104109 (2017), R. Sundararaman and Y. Ping, ‘First-principles electrostatic potentials for reliable alignment at interfaces and defects’
7. *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’
8. *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’
9. *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’
10. *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’
11. *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’
12. *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’
13. *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)’
14. *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’
15. *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’
16. *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’
18. *J. Chem. Phys.* **142**, 064107 (2015), R. Sundararaman and W.A. Goddard III, ‘The charge-asymmetric nonlocally-determined local-electric (CANDLE) solvation model’

19. *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*’
20. *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’
21. *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’
22. *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’
23. *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’
24. *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’
25. *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’
26. *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’
27. *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’
28. *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’
29. *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’
30. *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’
31. *IEEE Electron Device Letters* **32**, 414 (2011), J.M. Rubin, R. Sundararaman, M. Kim and S. Tiwari, ‘A Low-voltage Torsion Nanorelay’
32. *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, ‘A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices’
33. *IEEE Transactions on Magnetism*, **44**, 2351 (2008), G. Sinha, R. Sundararaman, and G. Singh, ‘Design Concepts of Optimized MRI Magnet’