Ravishankar Sundararaman

Rensselaer Polytechnic Institute
110 8th St, Troy, NY 12180
☎ *(518)276-6757*
✉ *sundar@rpi.edu*

Professional appointments

2016–present **Assistant Professor**, *Department of Materials Science and Engineering*, Rensselaer Polytechnic Institute.

2013–2016 **Postdoctoral fellow**, *Joint Center for Artifical Photosynthesis*, Lawrence Berkeley National Laboratory and California Institute of Technology.

Education

2013 **Ph.D. Physics**, *Cornell University*.

2007 **B.Sc. + M.Sc. Physics**, *Indian Institute of Technology, Kanpur*.

Awards and fellowships

2013–2015 Materials Postdoc Fellowship, Lawrence Berkeley National Laboratory

2012 Best poster at the 24th annual workshop on Electronic Structure methods

2007–2008 Cornell Graduate School Fellowship

2007 President's Gold Medal, IIT Kanpur

2002 Gold Medal at the 33rd International Physics Olympiad

2001 & 2002 Gold Medal at the Indian National Physics Olympiad

2000–2007 KVPY fellowship, Department of Science and Technology, Government of India

Open-source software contributions

JDFTx Software for joint density-functional theory, R. Sundararaman, K. Letchworth-Weaver, D. Gunceler, K.A. Schwarz and T.A. Arias, available from http://jdftx.sourceforge.net

VASPsol Solvation module for the VASP density-functional software, K. Matthew, R. Sundararaman, K. Letchworth-Weaver, T.A. Arias and R. Hennig, available from http://vaspsol.mse.ufl.edu

Invited talks

2017 'First-principles methods for modeling electrochemical processes', 254th ACS National Meeting, Washington DC (August 21, 2017)

'Plasmonic hot carriers: Towards material design', ACS 2017 Middle Atlantic Regional Meeting, Hershey, Pennsylvania (June 5, 2017)

'Material design for plasmonic and hot-carrier devices', Pacific Rim Conference on Ceramic and Glass Technology (PACRIM 12), Waikoloa, Hawaii (May 23, 2017)

'After the plasmon: designing materials to exploit non-equilibrium carriers', MRS Spring Meeting 2017, Phoenix (April 20, 2017)

2016 'Leaving the collective: plasmonics from a hot electron's point of view', International Center for Theoretical Sciences, Bengaluru, India

'Density-functional methods for electrochemistry and hot carrier dynamics', Department of Metallurgical and Materials Engineering, Indian Institute of Technology Madras, Chennai, India

'Leaving the collective: plasmonics from a hot electron's point of view', Department of Physics, Indian Institute of Technology Delhi, New Delhi, India

'Density-functional methods for electrochemistry and hot carrier dynamics', Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, India

'Leaving the collective: plasmonics from a hot electron's point of view', Tata Institute of Fundamental Research, Mumbai, India

'Plasmonic hot carrier dynamics: electronic structure perspectives', Workshop on physics of light-matter interactions and excited state dynamics, NG Next Basic Research Laboratory, Northrop Grumman corporation, Redondo Beach

'Electron interactions with liquids and light in nano-engineered energy conversion systems', Center for Nanoscale Materials, Argonne National Laboratory

'Electron interactions with liquids and light in nano-engineered energy conversion systems', Department of Materials Science, University of Wisconsin, Madison

2015 'First principles electrochemistry using joint density functional theory and continuum solvation methods', CAMS workshop on 'Enabling Methods for Materials Innovation from Quantum to Mesoscale', University of Florida, Gainesville

'Liquids, electrochemistry and plasmonics: from electronic structure to properties at the mesoscale', Department of Materials Science and Engineering, Penn State, University Park

2014 'Continuum solvation from joint density functional theory', Chemistry department, University of California, Riverside

2013 'Nonlocal polarizable continuum models from joint density functional theory', 25$^{\text{th}}$ annual workshop on Electronic Structure methods, College of William and Mary, Williamsburg

2011 'Accurate free energy functionals of liquid water for the Joint Density Functional description of solvated electronic systems', Theoretical chemistry division, Bhabha atomic research center, Mumbai, India

Teaching experience

Physics Department, Cornell University

Spring 2011 Laboratory instructor for Practical density-functional theory mini-course by Tomas Arias

Fall 2010 Grader for Statistical Physics graduate course by James Sethna

Spring 2009 Grader for Solid State Physics II graduate course by Chris Henley

Spring 2008 Laboratory instructor for Electronic Circuits undergraduate laboratory by Ivan Bazarov

Publications

2017 *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'

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'

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'

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'

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'

J. Chem. Phys. **146**, 104109 (2017), R. Sundararaman and Y. Ping, 'First-principles electrostatic potentials for reliable alignment at interfaces and defects'

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'

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'

2016 *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'

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'

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'

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'

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)'

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'

2015 *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'

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'

J. Chem. Phys. **142**, 214101 (2015), K.A. Schwarz, R. Sundararaman and T.A. Arias, 'Computationally efficient dielectric calculations of molecular crystals'

J. Chem. Phys. **142**, 064107 (2015), R. Sundararaman and W.A. Goddard III, 'The charge-asymmetric nonlocally-determined local-electric (CANDLE) solvation model'

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*'

2014 *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'

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'

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'

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'

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'

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'

2013 *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'

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'

2012 *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'

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'

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'

2011 *IEEE Electron Device Letters* **32**, 414 (2011), J.M. Rubin, R. Sundararaman, M. Kim and S. Tiwari, 'A Low-voltage Torsion Nanorelay'

2010 *Appl. Phys. Lett.* **96**, 023502 (2010), R. Sundararaman and S. Tiwari, 'A universal semiempirical model for the Fowler-Nordheim programming of charge trapping devices'

2008 *IEEE Transactions on Magnetics*, **44**, 2351 (2008), G. Sinha, R. Sundararaman, and G. Singh, 'Design Concepts of Optimized MRI Magnet'