Ravishankar Sundararaman

List of Publications by Year
in descending order

87 papers	7,441 citations	109321 35 h-index	53230 85 g-index
91 all docs	91 docs citations	91 times ranked	8527 citing authors

#	Article	IF	Citations
1	Implicit solvation model for density-functional study of nanocrystal surfaces and reaction pathways. Journal of Chemical Physics, 2014, 140, 084106.	3.0	1,676
2	Theoretical predictions for hot-carrier generation from surface plasmon decay. Nature Communications, 2014, 5, 5788.	12.8	600
3	Nonradiative Plasmon Decay and Hot Carrier Dynamics: Effects of Phonons, Surfaces, and Geometry. ACS Nano, 2016, 10, 957-966.	14.6	534
4	Mechanistic Explanation of the pH Dependence and Onset Potentials for Hydrocarbon Products from Electrochemical Reduction of CO on Cu (111). Journal of the American Chemical Society, 2016, 138, 483-486.	13.7	381
5	Plasmonic hot electron transport drives nano-localized chemistry. Nature Communications, 2017, 8, 14880.	12.8	328
6	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of Battery Electrode and Electrolyte. Nano Letters, 2014, 14, 1453-1459.	9.1	238
7	JDFTx: Software for joint density-functional theory. SoftwareX, 2017, 6, 278-284.	2.6	238
8	Plasmonic hot carrier dynamics in solid-state and chemical systems for energy conversion. Nanophotonics, 2016, 5, 96-111.	6.0	237
9	Grand canonical electronic density-functional theory: Algorithms and applications to electrochemistry. Journal of Chemical Physics, 2017, 146, 114104.	3.0	211
10	The importance of nonlinear fluid response in joint density-functional theory studies of battery systems. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 074005.	2.0	177
11	The charge-asymmetric nonlocally determined local-electric (CANDLE) solvation model. Journal of Chemical Physics, 2015, 142, 064107.	3.0	167
12	Electroless Formation of Hybrid Lithium Anodes for Fast Interfacial Ion Transport. Angewandte Chemie - International Edition, 2017, 56, 13070-13077.	13.8	151
13	Quantifying the role of surface plasmon excitation and hot carrier transport in plasmonic devices. Nature Communications, 2018, 9, 3394.	12.8	147
14	Ultrafast hot-hole injection modifies hot-electron dynamics in Au/p-GaN heterostructures. Nature Materials, 2020, 19, 1312-1318.	27.5	138
15	Ab initiophonon coupling and optical response of hot electrons in plasmonic metals. Physical Review B, 2016, 94, .	3.2	124
16	A chiral switchable photovoltaic ferroelectric 1D perovskite. Science Advances, 2020, 6, eaay4213.	10.3	119
17	Experimental and AbÂInitio Ultrafast Carrier Dynamics in Plasmonic Nanoparticles. Physical Review Letters, 2017, 118, 087401.	7.8	116
18	Plasmonic tunnel junctions for single-molecule redox chemistry. Nature Communications, 2017, 8, 994.	12.8	116

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19	Regularization of the Coulomb singularity in exact exchange by Wigner-Seitz truncated interactions: Towards chemical accuracy in nontrivial systems. Physical Review B, 2013, 87, .	3.2	102
20	The electrochemical interface in first-principles calculations. Surface Science Reports, 2020, 75, 100492.	7.2	89
21	Evaluating continuum solvation models for the electrode-electrolyte interface: Challenges and strategies for improvement. Journal of Chemical Physics, 2017, 146, 084111.	3.0	79
22	Lead-related quantum emitters in diamond. Physical Review B, 2019, 99, .	3.2	78
23	Hot carrier dynamics in plasmonic transition metal nitrides. Journal of Optics (United Kingdom), 2018, 20, 064001.	2.2	73
24	First-principles engineering of charged defects for two-dimensional quantum technologies. Physical Review Materials, 2017, 1, .	2.4	64
25	Formic acid oxidation on platinum: a simple mechanistic study. Physical Chemistry Chemical Physics, 2015, 17, 20805-20813.	2.8	56
26	Hot-Hole versus Hot-Electron Transport at Cu/GaN Heterojunction Interfaces. ACS Nano, 2020, 14, 5788-5797.	14.6	53
27	First-principles electrostatic potentials for reliable alignment at interfaces and defects. Journal of Chemical Physics, 2017, 146, 104109.	3.0	49
28	Dynamics and Spin-Valley Locking Effects in Monolayer Transition Metal Dichalcogenides. Nano Letters, 2018, 18, 5709-5715.	9.1	49
29	Spicing up continuum solvation models with SaLSA: The spherically averaged liquid susceptibility ansatz. Journal of Chemical Physics, 2015, 142, 054102.	3.0	48
30	Solvation effects on the band edge positions of photocatalysts from first principles. Physical Chemistry Chemical Physics, 2015, 17, 30499-30509.	2.8	47
31	The electrical resistivity of rough thin films: A model based on electron reflection at discrete step edges. Journal of Applied Physics, 2018, 123, .	2.5	44
32	Partial oxidation of step-bound water leads to anomalous pH effects on metal electrode step-edges. Physical Chemistry Chemical Physics, 2016, 18, 16216-16223.	2.8	40
33	Ultrafast Electron Dynamics in Single Aluminum Nanostructures. Nano Letters, 2019, 19, 3091-3097.	9.1	39
34	Improving the Accuracy of Atomistic Simulations of the Electrochemical Interface. Chemical Reviews, 2022, 122, 10651-10674.	47.7	39
35	Improving accuracy of electrochemical capacitance and solvation energetics in first-principles calculations. Journal of Chemical Physics, 2018, 148, 144105.	3.0	37
36	Microscopic origins of hydrodynamic transport in the type-II Weyl semimetal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WP</mml:mi><mml:mn>2</mml:mn></mml:msub></mm Physical Review B, 2018, 98, .	3.2	36

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37	Efficient classical density-functional theories of rigid-molecular fluids and a simplified free energy functional for liquid water. Computer Physics Communications, 2014, 185, 818-825.	7.5	35
38	Effects of Interlayer Coupling on Hotâ€Carrier Dynamics in Grapheneâ€Derived van der Waals Heterostructures. Advanced Optical Materials, 2017, 5, 1600914.	7.3	35
39	Room-temperature electrically switchable spinâ€“valley coupling in a van der Waals ferroelectric halide perovskite with persistent spin helix. Nature Photonics, 2022, 16, 529-537.	31.4	35
40	Materials for interconnects. MRS Bulletin, 2021, 46, 959-966.	3.5	33
41	Absence of diffuse double layer effect on the vibrational properties and oxidation of chemisorbed carbon monoxide on a Pt(111) electrode. Electrochimica Acta, 2018, 281, 127-132.	5.2	31
42	Electrochemical Capacitance of CO-Terminated Pt(111) Dominated by the COâ€“Solvent Gap. Journal of Physical Chemistry Letters, 2017, 8, 5344-5348.	4.6	30
43	Transport of hot carriers in plasmonic nanostructures. Physical Review Materials, 2019, 3, .	2.4	30
44	A computationally efficacious free-energy functional for studies of inhomogeneous liquid water. Journal of Chemical Physics, 2012, 137, 044107.	3.0	29
45	Weighted-density functionals for cavity formation and dispersion energies in continuum solvation models. Journal of Chemical Physics, 2014, 141, 134105.	3.0	26
46	Spin-phonon relaxation from a universal ab initio density-matrix approach. Nature Communications, 2020, 11, 2780.	12.8	26
47	A recipe for free-energy functionals of polarizable molecular fluids. Journal of Chemical Physics, 2014, 140, 144504.	3.0	24
48	Quantifying Uncertainties in Solvation Procedures for Modeling Aqueous Phase Reaction Mechanisms. Journal of Physical Chemistry A, 2021, 125, 154-164.	2.5	24
49	Increased rise time of electron temperature during adiabatic plasmon focusing. Nature Communications, 2017, 8, 1656.	12.8	23
50	Design Concepts of Optimized MRI Magnet. IEEE Transactions on Magnetics, 2008, 44, 2351-2360.	2.1	21
51	Layer dependence of defect charge transition levels in two-dimensional materials. Physical Review B, 2020, 101, .	3.2	19
52	Cubic Nonlinearity Driven Up-Conversion in High-Field Plasmonic Hot Carrier Systems. Journal of Physical Chemistry C, 2016, 120, 21056-21062.	3.1	17
53	Hydrodynamic and ballistic AC transport in two-dimensional Fermi liquids. Physical Review B, 2019, 99, .	3.2	17
54	Energy level alignment at semiconductorâ€“water interfaces from atomistic and continuum solvation models. RSC Advances, 2017, 7, 43660-43670.	3.6	16

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55	Substrate effects on charged defects in two-dimensional materials. Physical Review Materials, 2019, 3, .	2.4	16
56	A perspective on the data-driven design of polymer nanodielectrics. Journal Physics D: Applied Physics, 2020, 53, 333001.	2.8	15
57	Plasmonics in argentene. Physical Review Materials, 2020, 4, .	2.4	15
58	Framework for solvation in quantum Monte Carlo. Physical Review B, 2012, 85, .	3.2	14
59	Interdiffusion reliability and resistivity scaling of intermetallic compounds as advanced interconnect materials. Journal of Applied Physics, 2021, 129, .	2.5	14
60	Electron mobility in graphene without invoking the Dirac equation. American Journal of Physics, 2019, 87, 291-295.	0.7	13
61	Interfacial water asymmetry at ideal electrochemical interfaces. Journal of Chemical Physics, 2022, 156, 014705.	3.0	12
62	Electroless Formation of Hybrid Lithium Anodes for Fast Interfacial Ion Transport. Angewandte Chemie, 2017, 129, 13250-13257.	2.0	11
63	Quantification of functional crosslinker reaction kineticsviasuper-resolution microscopy of swollen microgels. Soft Matter, 2019, 15, 9336-9342.	2.7	11
64	Dielectric properties of polymer nanocomposite interphases from electrostatic force microscopy using machine learning. Materials Characterization, 2021, 173, 110909.	4.4	11
65	Near-Zero Negative Real Permittivity in Far Ultraviolet: Extending Plasmonics and Photonics with B1-MoN_x. Journal of Physical Chemistry C, 2019, 123, 21120-21129.	3.1	10
66	Effect of the density of states at the Fermi level on defect free energies and superconductivity: A case study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Nb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml: Physical Review B, 2021, 103, .	3.2	10
67	Ab initio ultrafast spin dynamics in solids. Physical Review B, 2021, 104, .	3.2	10
68	Ultralight Angstrom-Scale Optimal Optical Reflectors. ACS Photonics, 2018, 5, 384-389.	6.6	9
69	Plasmonic hot carriers scratch the surface. Trends in Chemistry, 2021, , .	8.5	9
70	A Low-Voltage Torsion Nanorelay. IEEE Electron Device Letters, 2011, 32, 414-416.	3.9	8
71	Temperature dependent electronâ€“phonon coupling of Au resolved via lattice dynamics measured with sub-picosecond infrared pulses. Journal of Applied Physics, 2021, 129, .	2.5	8
72	Resistivity scaling in epitaxial MAX-phase Ti4SiC3(0001) layers. Journal of Applied Physics, 2021, 130, .	2.5	8

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73	Giant Spin Lifetime Anisotropy and Spin-Valley Locking in Silicene and Germanene from First-Principles Density-Matrix Dynamics. Nano Letters, 2021, 21, 9594-9600.	9.1	7
74	Charge Trapping Devices Using a Bilayer Oxide Structure. Journal of Nanoscience and Nanotechnology, 2012, 12, 423-427.	0.9	5
75	First-principles identification of localized trap states in polymer nanocomposite interfaces. Journal of Materials Research, 2020, 35, 931-939.	2.6	5
76	Importance of bulk excitations and coherent electron-photon-phonon scattering in photoemission from PbTe(111): Ab initio theory with experimental comparisons. Physical Review B, 2021, 104, .	3.2	4
77	Electric fields and substrates dramatically accelerate spin relaxation in graphene. Physical Review B, 2022, 105, .	3.2	4
78	A single lithography vertical NEMS switch. , 2011, , .		2
79	Nanoscale Imaging of Lithium Ion Distribution During In Situ Operation of a Battery Electrode and Electrolyte. Microscopy and Microanalysis, 2014, 20, 1524-1525.	0.4	2
80	Computationally efficient dielectric calculations of molecular crystals. Journal of Chemical Physics, 2015, 142, 214101.	3.0	2
81	Designing High-Accuracy Permanent Magnets for Low-Power Magnetic Resonance Imaging. IEEE Transactions on Magnetics, 2018, 54, 1-9.	2.1	2
82	Resolving the Geometry/Charge Puzzle of the c(2 Ã— 2)-Cl Cu(100) Electrode. Journal of Physical Chemistry Letters, 2021, 12, 440-446.	4.6	2
83	Behavior of Linear and Nonlinear Dimensionality Reduction for Collective Variable Identification of Small Molecule Solution-Phase Reactions. Journal of Chemical Theory and Computation, 2022, 18, 1286-1296.	5.3	2
84	Coupled Electromagnetic and Reaction Kinetics Simulation of Super-Resolution Interference Lithography. Journal of Physical Chemistry B, 2020, 124, 7717-7724.	2.6	1
85	(Invited) Combining Machine Learning, DFT, EFM, and Modeling to Design Nanodielectric Behavior. ECS Transactions, 2022, 108, 51-60.	0.5	1
86	A universal semiempirical model for the Fowlerâ€“Nordheim programming of charge trapping devices. Applied Physics Letters, 2010, 96, 023502.	3.3	0
87	Trap dynamics of hot electrons in metalâ€“insulatorâ€“metal plasmonic structures for ultra-fast optoelectronics. Journal of Applied Physics, 2022, 131, 194501.	2.5	0