

Sergey N Rashkeev

List of Publications by Year in descending order

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91
papers

3,374
citations

147801

31
h-index

149698

56
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93
all docs

93
docs citations

93
times ranked

4002
citing authors

#	ARTICLE	IF	CITATIONS
1	Efficientab initiomethod for the calculation of frequency-dependent second-order optical response in semiconductors. <i>Physical Review B</i> , 1998, 57, 3905-3919.	3.2	371
2	Dopants adsorbed as single atoms prevent degradation of catalyts. <i>Nature Materials</i> , 2004, 3, 143-146.	27.5	199
3	Thermal stability and catalytic activity of gold nanoparticles supported on silica. <i>Journal of Catalysis</i> , 2009, 262, 92-101.	6.2	170
4	Defect Generation by Hydrogen at the Si-SiO ₂ Interface. <i>Physical Review Letters</i> , 2001, 87, 165506.	7.8	159
5	Electronic Band Structure of SiC Polytypes: A Discussion of Theory and Experiment. <i>Physica Status Solidi (B): Basic Research</i> , 1997, 202, 5-33.	1.5	150
6	Resonant Raman scattering inYBa ₂ Cu ₃ O ₇ : Band theory and experiment. <i>Physical Review Letters</i> , 1990, 65, 3048-3051.	7.8	129
7	COVID-19 (SARS-CoV-2) outbreak monitoring using wastewater-based epidemiology in Qatar. <i>Science of the Total Environment</i> , 2021, 774, 145608.	8.0	120
8	Hydrogen Bonding and Stability of Hybrid Organicâ€“Inorganic Perovskites. <i>ChemSusChem</i> , 2016, 9, 2648-2655.	6.8	109
9	Shear-strain-induced chemical reactivity of layered molecular crystals. <i>Applied Physics Letters</i> , 2007, 90, 151913.	3.3	97
10	Second-harmonic generation and birefringence of some ternary pnictide semiconductors. <i>Physical Review B</i> , 1999, 59, 2737-2748.	3.2	87
11	Quantitative theory of superconductivity in dopedC ₆₀ . <i>Physical Review B</i> , 1992, 45, 5114-5117.	3.2	79
12	First-principles calculations of the optical properties of metals. <i>Journal of Physics F: Metal Physics</i> , 1988, 18, 833-849.	1.6	75
13	Origin of Anomalous Pt-Pt Distances in the Pt/Alumina Catalytic System. <i>ChemPhysChem</i> , 2004, 5, 1893-1897.	2.1	68
14	Atomic-scale mechanisms of oxygen electrode delamination in solid oxide electrolyzer cells. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 1280-1291.	7.1	59
15	Microscopic studies of the optical spectra ofYBa ₂ Cu ₃ O ₇ . <i>Physical Review Letters</i> , 1989, 63, 1880-1883.	7.8	54
16	Optical-absorption bands in the 1â€“3 eV range inn-type SiC polytypes. <i>Physical Review B</i> , 1999, 59, 12890-12899.	3.2	54
17	Interplay of Decomposition Mechanisms at Shear-Strain Interface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 17-20.	3.1	49
18	Second-harmonic generation in SiC polytypes. <i>Physical Review B</i> , 1998, 57, 9705-9715.	3.2	47

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19	Catalytic activity of supported metal particles for sulfuric acid decomposition reaction. <i>Catalysis Today</i> , 2009, 139, 291-298.	4.4	47
20	Negative bias-temperature instabilities in metal-oxide-silicon devices with SiO ₂ and SiO _x N _y /HfO ₂ gate dielectrics. <i>Applied Physics Letters</i> , 2004, 84, 4394-4396.	3.3	46
21	Atomic Scale Mechanism of the Transformation of γ -Alumina to δ -Alumina. <i>Physical Review Letters</i> , 2002, 89, 235501.	7.8	45
22	Ethanol oxidation on metal oxide-supported platinum catalysts. <i>Catalysis Today</i> , 2009, 147, 107-114.	4.4	43
23	Enhancing Intrinsic Stability of Hybrid Perovskite Solar Cell by Strong, yet Balanced, Electronic Coupling. <i>Scientific Reports</i> , 2016, 6, 30305.	3.3	42
24	Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in CH ₃ NH ₃ PbI ₃ Solar Cell High Performance. <i>Scientific Reports</i> , 2015, 5, 11467.	3.3	41
25	X-ray absorption, glancing-angle reflectivity, and theoretical study of the N K- and Ga M _{2,3} -edge spectra in GaN. <i>Physical Review B</i> , 1997, 55, 2612-2622.	3.2	40
26	An efficient descriptor model for designing materials for solar cells. <i>Npj Computational Materials</i> , 2015, 1, .	8.7	39
27	Electronic excitations and decomposition of 1,1-diamino-2,2-dinitroethylene. <i>Applied Physics Letters</i> , 2003, 82, 1371-1373.	3.3	38
28	Oxidation and hydrogen uptake in zirconium, Zircaloy-2 and Zircaloy-4: Computational thermodynamics and ab initio calculations. <i>Journal of Nuclear Materials</i> , 2014, 444, 65-75.	2.7	38
29	Fermi-surface and low-energy excitation spectrum of YBa ₂ Cu ₃ O ₇ : Role of the Ba-O plane. <i>Physical Review B</i> , 1992, 45, 5103-5106.	3.2	36
30	Dual behavior of H ⁺ at Si-SiO ₂ interfaces: Mobility versus trapping. <i>Applied Physics Letters</i> , 2002, 81, 1839-1841.	3.3	35
31	Self-Accelerated Mechanochemistry in Nitroarenes. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 363-367.	4.6	35
32	Hydrogen bonding: a mechanism for tuning electronic and optical properties of hybrid organic-inorganic frameworks. <i>Npj Computational Materials</i> , 2016, 2, .	8.7	32
33	Electronic transport in nanoscale contacts with rough boundaries. <i>Physical Review B</i> , 1996, 53, 13074-13085.	3.2	31
34	Electronic transport in organometallic perovskite CH ₃ NH ₃ PbI ₃ : The role of organic cation orientations. <i>Applied Physics Letters</i> , 2016, 108, 053901.	3.3	28
35	Sp ² carbon embedded in Al-6061 and Al-7075 alloys in the form of crystalline graphene nanoribbons. <i>Carbon</i> , 2016, 107, 56-66.	10.3	28
36	Nonspherical rigid-muffin-tin calculations of electron-phonon coupling in high-T _c perovskites. <i>Physical Review B</i> , 1990, 42, 366-370.	3.2	27

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37	Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice. <i>Advanced Functional Materials</i> , 2015, 25, 4768-4777.	14.9	27
38	Extending Shannon's ionic radii database using machine learning. <i>Physical Review Materials</i> , 2021, 5, .	2.4	27
39	Electronic Raman continuum for $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$: Effects of inelastic scattering and interband transitions. <i>Physical Review B</i> , 1993, 47, 11603-11606.	3.2	25
40	Hydrogen passivation and activation of oxygen complexes in silicon. <i>Applied Physics Letters</i> , 2001, 78, 1571-1573.	3.3	23
41	Modification of Au/TiO_2 Nanosystems by SiO_2 Monolayers: Toward the Control of the Catalyst Activity and Stability. <i>Journal of Physical Chemistry C</i> , 2010, 114, 2996-3002.	3.1	23
42	Low-energy interband transitions in $\text{YBa}_2\text{Cu}_3\text{O}_7$. <i>Physical Review B</i> , 1992, 46, 11232-11235.	3.2	21
43	Strong enhancement of second-order response coefficients in tellurium containing $\text{Ag}^{\text{III}}\text{VI}_2$ compounds. <i>Applied Physics Letters</i> , 2000, 77, 190-192.	3.3	20
44	First-principles calculations of second-order optical response functions in chalcopyrite semiconductors. <i>Journal of Physics and Chemistry of Solids</i> , 2003, 64, 1615-1619.	4.0	20
45	Role of Electronic versus Atomic Relaxations in Stokes Shifts at Defects in Solids. <i>Physical Review Letters</i> , 2003, 91, 226402.	7.8	20
46	Structural Stability and Catalytic Activity of Lanthanum-Based Perovskites. <i>Journal of Physical Chemistry C</i> , 2011, 115, 8709-8715.	3.1	20
47	Polarization switching in optical microsphere resonator. <i>Applied Physics Letters</i> , 2002, 80, 3503-3505.	3.3	19
48	A comprehensive risk assessment of toxic elements in international brands of face foundation powders. <i>Environmental Research</i> , 2021, 192, 110274.	7.5	19
49	Band gap tuning in aluminum doped two-dimensional hexagonal boron nitride. <i>Materials Chemistry and Physics</i> , 2020, 250, 123176.	4.0	19
50	Electronic structure, ferromagnetism, and EELS spectra of crystalline alloys Fe_nB and Ni_nB ($n=1,2,3$): Aspects of universal behavior. <i>Physical Review B</i> , 1993, 48, 6260-6270.	3.2	18
51	Electronic structure, Schottky barrier, and optical spectra of the SiC/TiC {111} interface. <i>Physical Review B</i> , 1997, 55, 16472-16486.	3.2	18
52	Hydrogen-Induced Initiation of Corrosion in Aluminum. <i>Journal of Physical Chemistry C</i> , 2007, 111, 7175-7178.	3.1	18
53	Effects of Hydrogen on the Radiation Response of Bipolar Transistors: Experiment and Modeling. <i>IEEE Transactions on Nuclear Science</i> , 2008, 55, 3039-3045.	2.0	18
54	Molecular Mechanisms of Shear Strain Sensitivity of the Energetic Crystals DADNE and TATB. <i>Journal of Energetic Materials</i> , 2010, 28, 66-77.	2.0	18

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55	Effects of thermophoresis on dust accumulation on solar panels. <i>Solar Energy</i> , 2020, 211, 412-417.	6.1	18
56	Multi-Scale Simulation of Radiation Effects in Electronic Devices. <i>IEEE Transactions on Nuclear Science</i> , 2008, 55, 1891-1902.	2.0	17
57	Defect states at organic–inorganic interfaces: Insight from first principles calculations for pentaerythritol tetranitrate on MgO surface. <i>Surface Science</i> , 2015, 637-638, 19-28.	1.9	17
58	Intrinsic stability enhancement and ionic migration reduction by fluorinated cations incorporated in hybrid lead halide perovskites. <i>Journal of Materials Chemistry C</i> , 2019, 7, 5299-5306.	5.5	17
59	Breakdown of conductance quantization in quantum point contacts with realistic impurity potentials. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 6253-6270.	1.8	15
60	Control of oxygen delamination in solid oxide electrolyzer cells via modifying operational regime. <i>Applied Physics Letters</i> , 2011, 99, 173506.	3.3	15
61	Controlling chromium vaporization from interconnects with nickel coatings in solid oxide devices. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 15031-15038.	7.1	15
62	Universality in Electronic Structure and EELS Spectra of Fe-B and Ni-B Crystalline and Amorphous Systems. <i>Europhysics Letters</i> , 1994, 26, 43-49.	2.0	11
63	Solar Cell Materials by Design: Hybrid Pyroxene Corner-Sharing VO ₄ Tetrahedral Chains. <i>ChemSusChem</i> , 2017, 10, 1931-1942.	6.8	10
64	Tunable high workfunction contacts: Doped graphene. <i>Applied Surface Science</i> , 2020, 509, 144893.	6.1	10
65	Doped Nickel Oxide Carrier-Selective Contact for Silicon Solar Cells. <i>IEEE Journal of Photovoltaics</i> , 2021, 11, 1176-1187.	2.5	10
66	Two-color optical technique for characterization of x-ray radiation-enhanced electron transport in SiO ₂ . <i>Journal of Applied Physics</i> , 2003, 93, 1865-1870.	2.5	9
67	Highly accurate machine learning prediction of crystal point groups for ternary materials from chemical formula. <i>Scientific Reports</i> , 2022, 12, 1577.	3.3	9
68	The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O ₃ Complex Perovskites. <i>ECS Transactions</i> , 2011, 35, 2077-2084.	0.5	8
69	Ultra-high temperature steam corrosion of complex silicates for nuclear applications: A computational study. <i>Journal of Nuclear Materials</i> , 2014, 444, 56-64.	2.7	8
70	Photochemistry of the α -Al ₂ O ₃ -PETN Interface. <i>Molecules</i> , 2016, 21, 289.	3.8	8
71	Radiation-induced acceptor deactivation in bipolar devices: Effects of electric field. <i>Applied Physics Letters</i> , 2003, 83, 4646-4648.	3.3	7
72	Achieving tunable chemical reactivity through photo-initiation of energetic materials at metal oxide surfaces. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25284-25296.	2.8	6

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73	Interaction of gas molecules with crystalline polymer separation membranes: Atomic-scale modeling and first-principles calculations. <i>Journal of Membrane Science</i> , 2011, 384, 176-183.	8.2	5
74	Effect of Affinity Discontinuity on Heterojunction p-i-n Solar Cell Performance. <i>IEEE Journal of Photovoltaics</i> , 2020, 10, 458-466.	2.5	5
75	Strain-rate sensitivity limit diagrams and plastic instabilities in a 6xxx series aluminum alloy Part I: Analysis of temporal stress-strain serrations. <i>Computational Materials Science</i> , 2002, 24, 295-309.	3.0	4
76	Beryllium Adsorption at Transition Aluminas: Implications for Environmental Science and Oxidation of Aluminum Alloys. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14208-14212.	3.1	4
77	Enhancing the electronic dimensionality of hybrid organic-inorganic frameworks by hydrogen bonded molecular cations. <i>Materials Horizons</i> , 2019, 6, 1187-1196.	12.2	4
78	Single-Atom Sensitivity for Solving Catalysis Problems. <i>Microscopy and Microanalysis</i> , 2004, 10, 460-461.	0.4	3
79	Fischer-Tropsch Synthesis over Supported Pt-Mo Catalyst: Toward Bimetallic Catalyst Optimization. <i>Journal of Physical Chemistry C</i> , 2013, 117, 4450-4458.	3.1	3
80	A simple reaction-diffusion model for initial stages of biofouling in reverse osmosis membranes. <i>Environmental Research</i> , 2020, 190, 110000.	7.5	3
81	Bifacial Schottky-Junction Plasmonic-Based Solar Cell. <i>Energy Technology</i> , 2020, 8, 1901280.	3.8	3
82	Melting Phase Transitions and Catalytic Activity of Bilayer Gold Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10517-10520.	3.1	2
83	Improved Photoactivity of Pyroxene Silicates by Cation Substitutions. <i>ChemPhysChem</i> , 2018, 19, 943-953.	2.1	2
84	Spin/carrier dynamics at semiconductor interfaces using intense, tunable, ultra-fast lasers. <i>Physica Status Solidi (B): Basic Research</i> , 2003, 240, 490-499.	1.5	1
85	HYDROGEN AT THE Si/SiO ₂ INTERFACE: FROM ATOMIC-SCALE CALCULATIONS TO ENGINEERING MODELS. <i>International Journal of High Speed Electronics and Systems</i> , 2004, 14, 575-580.	0.7	1
86	Performance, Reliability, Radiation Effects, and Aging Issues in Microelectronics - From Atomic-Scale Physics to Engineering-Level Modeling. <i>ECS Transactions</i> , 2009, 19, 319-337.	0.5	1
87	Oxychalcogenide Perovskite Solar Cells: A Multiscale Design Approach. <i>Energy Technology</i> , 2020, 8, 1900766.	3.8	1
88	Optimized Ni _{1-x} Al _x O hole transport layer for silicon solar cells. <i>RSC Advances</i> , 2020, 10, 22377-22386.	3.6	1
89	Synthetic Alloys: Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice (<i>Adv. Funct. Mater.</i> 30/2015). <i>Advanced Functional Materials</i> , 2015, 25, 4746-4746.	14.9	0
90	Growth of Hybrid Perovskites (HP) Light Harvesting Layer and TiO ₂ Electron Transport Material for Solar Cells Application. , 2016, , .		0

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91	Achieving tunable sensitivity in composite high-energy density materials. AIP Conference Proceedings, 2017, , .	0.4	0