Sergey N Rashkeev

List of Publications by Year
in descending order

91	3,374	147801 31	149698 56
papers	citations	h-index	g-index

93	93	93	4002
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Highly accurate machine learning prediction of crystal point groups for ternary materials from chemical formula. Scientific Reports, 2022, 12, 1577.	3.3	9
2	A comprehensive risk assessment of toxic elements in international brands of face foundation powders. Environmental Research, 2021, 192, 110274.	7.5	19
3	Extending Shannon's ionic radii database using machine learning. Physical Review Materials, 2021, 5, .	2.4	27
4	COVID-19 (SARS-CoV-2) outbreak monitoring using wastewater-based epidemiology in Qatar. Science of the Total Environment, 2021, 774, 145608.	8.0	120
5	Doped Nickel Oxide Carrier-Selective Contact for Silicon Solar Cells. IEEE Journal of Photovoltaics, 2021, 11, 1176-1187.	2.5	10
6	Oxychalcogenide Perovskite Solar Cells: A Multiscale Design Approach. Energy Technology, 2020, 8, 1900766.	3.8	1
7	Tunable high workfunction contacts: Doped graphene. Applied Surface Science, 2020, 509, 144893.	6.1	10
8	Effects of thermophoresis on dust accumulation on solar panels. Solar Energy, 2020, 211, 412-417.	6.1	18
9	Achieving tunable chemical reactivity through photo-initiation of energetic materials at metal oxide surfaces. Physical Chemistry Chemical Physics, 2020, 22, 25284-25296.	2.8	6
10	A simple reaction-diffusion model for initial stages of biofouling in reverse osmosis membranes. Environmental Research, 2020, 190, 110000.	7.5	3
11	Optimized Ni_{1â^'x}Al_xO hole transport layer for silicon solar cells. RSC Advances, 2020, 10, 22377-22386.	3.6	1
12	Bifacial Schottkyâ€Junction Plasmonicâ€Based Solar Cell. Energy Technology, 2020, 8, 1901280.	3.8	3
13	Effect of Affinity Discontinuity on Heterojunction p-i-n Solar Cell Performance. IEEE Journal of Photovoltaics, 2020, 10, 458-466.	2.5	5
14	Band gap tuning in aluminum doped two-dimensional hexagonal boron nitride. Materials Chemistry and Physics, 2020, 250, 123176.	4.0	19
15	Intrinsic stability enhancement and ionic migration reduction by fluorinated cations incorporated in hybrid lead halide perovskites. Journal of Materials Chemistry C, 2019, 7, 5299-5306.	5.5	17
16	Enhancing the electronic dimensionality of hybrid organicâ€“inorganic frameworks by hydrogen bonded molecular cations. Materials Horizons, 2019, 6, 1187-1196.	12.2	4
17	Improved Photoactivity of Pyroxene Silicates by Cation Substitutions. ChemPhysChem, 2018, 19, 943-953.	2.1	2
18	Achieving tunable sensitivity in composite high-energy density materials. AIP Conference Proceedings, 2017, , .	0.4	0

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19	Solar Cell Materials by Design: Hybrid Pyroxene Cornerâ€Sharing VO₄ Tetrahedral Chains. ChemSusChem, 2017, 10, 1931-1942.	6.8	10
20	Photochemistry of the Î±-Al2O3-PETN Interface. Molecules, 2016, 21, 289.	3.8	8
21	Growth of Hybrid Perovskites (HP) Light Harvesting Layer and TiO 2 Electron Transport Material for Solar Cells Application. , 2016, , .		0
22	Electronic transport in organometallic perovskite CH₃NH₃PbI₃: The role of organic cation orientations. Applied Physics Letters, 2016, 108, 053901.	3.3	28
23	Hydrogen Bonding and Stability of Hybrid Organicâ€“Inorganic Perovskites. ChemSusChem, 2016, 9, 2648-2655.	6.8	109
24	Hydrogen bonding: a mechanism for tuning electronic and optical properties of hybrid organicâ€“inorganic frameworks. Npj Computational Materials, 2016, 2, .	8.7	32
25	Enhancing Intrinsic Stability of Hybrid Perovskite Solar Cell by Strong, yet Balanced, Electronic Coupling. Scientific Reports, 2016, 6, 30305.	3.3	42
26	Sp2 carbon embedded in Al-6061 and Al-7075 alloys in the form of crystalline graphene nanoribbons. Carbon, 2016, 107, 56-66.	10.3	28
27	Synthetic Alloys: Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice (Adv. Funct. Mater. 30/2015). Advanced Functional Materials, 2015, 25, 4746-4746.	14.9	0
28	An efficient descriptor model for designing materials for solar cells. Npj Computational Materials, 2015, 1, .	8.7	39
29	Synthetic Crystals of Silver with Carbon: 3D Epitaxy of Carbon Nanostructures in the Silver Lattice. Advanced Functional Materials, 2015, 25, 4768-4777.	14.9	27
30	Defect states at organicâ€“inorganic interfaces: Insight from first principles calculations for pentaerythritol tetranitrate on MgO surface. Surface Science, 2015, 637-638, 19-28.	1.9	17
31	Domain Walls Conductivity in Hybrid Organometallic Perovskites and Their Essential Role in CH3NH3PbI3 Solar Cell High Performance. Scientific Reports, 2015, 5, 11467.	3.3	41
32	Controlling chromium vaporization from interconnects with nickel coatings in solid oxide devices. International Journal of Hydrogen Energy, 2014, 39, 15031-15038.	7.1	15
33	Oxidation and hydrogen uptake in zirconium, Zircaloy-2 and Zircaloy-4: Computational thermodynamics and ab initio calculations. Journal of Nuclear Materials, 2014, 444, 65-75.	2.7	38
34	Ultra-high temperature steam corrosion of complex silicates for nuclear applications: A computational study. Journal of Nuclear Materials, 2014, 444, 56-64.	2.7	8
35	Fischerâ€“Tropsch Synthesis over Supported Ptâ€“Mo Catalyst: Toward Bimetallic Catalyst Optimization. Journal of Physical Chemistry C, 2013, 117, 4450-4458.	3.1	3
36	Atomic-scale mechanisms of oxygen electrode delamination in solid oxide electrolyzer cells. International Journal of Hydrogen Energy, 2012, 37, 1280-1291.	7.1	59

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37	Control of oxygen delamination in solid oxide electrolyzer cells via modifying operational regime. Applied Physics Letters, 2011, 99, 173506.	3.3	15
38	Structural Stability and Catalytic Activity of Lanthanum-Based Perovskites. Journal of Physical Chemistry C, 2011, 115, 8709-8715.	3.1	20
39	Interaction of gas molecules with crystalline polymer separation membranes: Atomic-scale modeling and first-principles calculations. Journal of Membrane Science, 2011, 384, 176-183.	8.2	5
40	The Structural Disorder and Lattice Stability of (Ba,Sr)(Co,Fe)O₃ Complex Perovskites. ECS Transactions, 2011, 35, 2077-2084.	0.5	8
41	Molecular Mechanisms of Shear Strain Sensitivity of the Energetic Crystals DADNE and TATB. Journal of Energetic Materials, 2010, 28, 66-77.	2.0	18
42	Self-Accelerated Mechanochemistry in Nitroarenes. Journal of Physical Chemistry Letters, 2010, 1, 363-367.	4.6	35
43	Beryllium Adsorption at Transition Aluminas: Implications for Environmental Science and Oxidation of Aluminum Alloys. Journal of Physical Chemistry C, 2010, 114, 14208-14212.	3.1	4
44	Modification of Au/TiO₂ Nanosystems by SiO₂ Monolayers: Toward the Control of the Catalyst Activity and Stability. Journal of Physical Chemistry C, 2010, 114, 2996-3002.	3.1	23
45	Performance, Reliability, Radiation Effects, and Aging Issues in Microelectronics - From Atomic-Scale Physics to Engineering-Level Modeling. ECS Transactions, 2009, 19, 319-337.	0.5	1
46	Thermal stability and catalytic activity of gold nanoparticles supported on silica. Journal of Catalysis, 2009, 262, 92-101.	6.2	170
47	Catalytic activity of supported metal particles for sulfuric acid decomposition reaction. Catalysis Today, 2009, 139, 291-298.	4.4	47
48	Ethanol oxidation on metal oxide-supported platinum catalysts. Catalysis Today, 2009, 147, 107-114.	4.4	43
49	Melting Phase Transitions and Catalytic Activity of Bilayer Gold Nanoclusters. Journal of Physical Chemistry C, 2009, 113, 10517-10520.	3.1	2
50	Interplay of Decomposition Mechanisms at Shear-Strain Interface. Journal of Physical Chemistry C, 2009, 113, 17-20.	3.1	49
51	Effects of Hydrogen on the Radiation Response of Bipolar Transistors: Experiment and Modeling. IEEE Transactions on Nuclear Science, 2008, 55, 3039-3045.	2.0	18
52	Multi-Scale Simulation of Radiation Effects in Electronic Devices. IEEE Transactions on Nuclear Science, 2008, 55, 1891-1902.	2.0	17
53	Shear-strain-induced chemical reactivity of layered molecular crystals. Applied Physics Letters, 2007, 90, 151913.	3.3	97
54	Hydrogen-Induced Initiation of Corrosion in Aluminum. Journal of Physical Chemistry C, 2007, 111, 7175-7178.	3.1	18

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55	Negative bias-temperature instabilities in metalâ€“oxideâ€“silicon devices with SiO2 and SiOxNy/HfO2 gate dielectrics. Applied Physics Letters, 2004, 84, 4394-4396.	3.3	46
56	HYDROGEN AT THE Si/SiO2 INTERFACE: FROM ATOMIC-SCALE CALCULATIONS TO ENGINEERING MODELS. International Journal of High Speed Electronics and Systems, 2004, 14, 575-580.	0.7	1
57	Dopants adsorbed as single atoms prevent degradation of catalysts. Nature Materials, 2004, 3, 143-146.	27.5	199
58	Origin of Anomalous Pt-Pt Distances in the Pt/Alumina Catalytic System. ChemPhysChem, 2004, 5, 1893-1897.	2.1	68
59	Single-Atom Sensitivity for Solving Catalysis Problems. Microscopy and Microanalysis, 2004, 10, 460-461.	0.4	3
60	First-principles calculations of second-order optical response functions in chalcopyrite semiconductors. Journal of Physics and Chemistry of Solids, 2003, 64, 1615-1619.	4.0	20
61	Spin/carrier dynamics at semiconductor interfaces using intense, tunable, ultra-fast lasers. Physica Status Solidi (B): Basic Research, 2003, 240, 490-499.	1.5	1
62	Role of Electronic versus Atomic Relaxations in Stokes Shifts at Defects in Solids. Physical Review Letters, 2003, 91, 226402.	7.8	20
63	Two-color optical technique for characterization of x-ray radiation-enhanced electron transport in SiO2. Journal of Applied Physics, 2003, 93, 1865-1870.	2.5	9
64	Radiation-induced acceptor deactivation in bipolar devices: Effects of electric field. Applied Physics Letters, 2003, 83, 4646-4648.	3.3	7
65	Electronic excitations and decomposition of 1,1-diamino-2,2-dinitroethylene. Applied Physics Letters, 2003, 82, 1371-1373.	3.3	38
66	Dual behavior of H+ at Siâ€“SiO2 interfaces: Mobility versus trapping. Applied Physics Letters, 2002, 81, 1839-1841.	3.3	35
67	Polarization switching in optical microsphere resonator. Applied Physics Letters, 2002, 80, 3503-3505.	3.3	19
68	Strain-rate sensitivity limit diagrams and plastic instabilities in a 6xxx series aluminum alloy Part I: Analysis of temporal stressâ€“strain serrations. Computational Materials Science, 2002, 24, 295-309.	3.0	4
69	Atomic Scale Mechanism of the Transformation ofÎ³-Alumina toÎ¸-Alumina. Physical Review Letters, 2002, 89, 235501.	7.8	45
70	Defect Generation by Hydrogen at the Si-SiO2Interface. Physical Review Letters, 2001, 87, 165506.	7.8	159
71	Hydrogen passivation and activation of oxygen complexes in silicon. Applied Physics Letters, 2001, 78, 1571-1573.	3.3	23
72	Strong enhancement of second-order response coefficients in tellurium containing Agâ€“IIIâ€“VI2 compounds. Applied Physics Letters, 2000, 77, 190-192.	3.3	20

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73	Optical-absorption bands in the 1â€“3 eV range inn-type SiC polytypes. Physical Review B, 1999, 59, 12890-12899.	3.2	54
74	Second-harmonic generation and birefringence of some ternary pnictide semiconductors. Physical Review B, 1999, 59, 2737-2748.	3.2	87
75	Second-harmonic generation in SiC polytypes. Physical Review B, 1998, 57, 9705-9715.	3.2	47
76	Efficientab initiomethod for the calculation of frequency-dependent second-order optical response in semiconductors. Physical Review B, 1998, 57, 3905-3919.	3.2	371
77	X-ray absorption, glancing-angle reflectivity, and theoretical study of the N K- and GaM2,3-edge spectra in GaN. Physical Review B, 1997, 55, 2612-2622.	3.2	40
78	Electronic structure, Schottky barrier, and optical spectra of the SiC/TiC {111} interface. Physical Review B, 1997, 55, 16472-16486.	3.2	18
79	Electronic Band Structure of SiC Polytypes: A Discussion of Theory and Experiment. Physica Status Solidi (B): Basic Research, 1997, 202, 5-33.	1.5	150
80	Electronic transport in nanoscale contacts with rough boundaries. Physical Review B, 1996, 53, 13074-13085.	3.2	31
81	Breakdown of conductance quantization in quantum point contacts with realistic impurity potentials. Journal of Physics Condensed Matter, 1995, 7, 6253-6270.	1.8	15
82	Universality in Electronic Structure and EELS Spectra of Fe-B and Ni-B Crystalline and Amorphous Systems. Europhysics Letters, 1994, 26, 43-49.	2.0	11
83	Electronic Raman continuum forYBa2Cu3O7â^'Î´: Effects of inelastic scattering and interband transitions. Physical Review B, 1993, 47, 11603-11606.	3.2	25
84	Electronic structure, ferromagnetism, and EELS spectra of crystalline alloysFenB andNinB (n=1,2,3): Aspects of universal behavior. Physical Review B, 1993, 48, 6260-6270.	3.2	18
85	Fermi-surface and low-energy excitation spectrum ofYBa2Cu3O7: Role of the Ba-O plane. Physical Review B, 1992, 45, 5103-5106.	3.2	36
86	Quantitative theory of superconductivity in dopedC60. Physical Review B, 1992, 45, 5114-5117.	3.2	79
87	Low-energy interband transitions inYBa2Cu3O7. Physical Review B, 1992, 46, 11232-11235.	3.2	21
88	Resonant Raman scattering inYBa2Cu3O7: Band theory and experiment. Physical Review Letters, 1990, 65, 3048-3051.	7.8	129
89	Nonspherical rigid-muffin-tin calculations of electron-phonon coupling in high-Tcperovskites. Physical Review B, 1990, 42, 366-370.	3.2	27
90	Microscopic studies of the optical spectra ofYBa2Cu3O7. Physical Review Letters, 1989, 63, 1880-1883.	7.8	54

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91	First-principles calculations of the optical properties of metals. Journal of Physics F: Metal Physics, 1988, 18, 833-849.	1.6	75