Arkady Krasheninnikov

List of Publications by Year
in descending order

246	26,941	8732 75	5965 160
papers	citations	h-index	g-index

259	259	259	24237
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Efficient Calculation of the Lattice Thermal Conductivity by Atomistic Simulations with Ab Initio Accuracy. Advanced Theory and Simulations, 2022, 5, .	1.3	14
2	Data-Driven Quest for Two-Dimensional Non-van der Waals Materials. Nano Letters, 2022, 22, 989-997.	4.5	35
3	Edge and Pointâ€Defect Induced Electronic and Magnetic Properties in Monolayer PtSe₂. Advanced Functional Materials, 2022, 32, .	7.8	21
4	Threshold Ion Energies for Creating Defects in 2D Materials from First-Principles Calculations: Chemical Interactions Are Important. Journal of Physical Chemistry Letters, 2022, 13, 514-519.	2.1	13
5	Physics and theory of defects in 2D materials: the role of reduced dimensionality. , 2022, , 7-41.		5
6	Two-dimensional materials under ion irradiation: from defect production to structure and property engineering. , 2022, , 259-301.		2
7	Self-Driven Broadband Photodetectors Based on MoSe₂/FePS₃ van der Waals nâ€“p Type-II Heterostructures. ACS Applied Materials & Interfaces, 2022, 14, 11927-11936.	4.0	35
8	Compact Laser Devices for Measuring Airborne Microparticle Concentrations and Their Application at the Geophysical Monitoring Center of the Sadovsky Institute of Dynamics of Geospheres, Russian Academy of Sciences. Seismic Instruments, 2022, 58, 235-243.	0.0	0
9	Controlling Stoichiometry in Ultrathin van der Waals Films: PtTe₂, Pt₂Te₃, Pt₃Te₄, and Pt₂Te₂. ACS Nano, 2022, 16, 9908-9919.	7.3	8
10	Low-energy Se ion implantation in MoS2 monolayers. Npj 2D Materials and Applications, 2022, 6, .	3.9	11
11	Mirror twin boundaries in MoSe2 monolayers as one dimensional nanotemplates for selective water adsorption. Nanoscale, 2021, 13, 1038-1047.	2.8	11
12	Robust Magnetoelectric Effect in the Decorated Graphene/In₂Se₃ Heterostructure. ACS Applied Materials & Interfaces, 2021, 13, 3033-3039.	4.0	15
13	Formation of Highly Doped Nanostripes in 2D Transition Metal Dichalcogenides via a Dislocation Climb Mechanism. Advanced Materials, 2021, 33, e2007819.	11.1	13
14	Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering. Science Advances, 2021, 7, .	4.7	51
15	Photoluminescence line shapes for color centers in silicon carbide from density functional theory calculations. Physical Review B, 2021, 103, .	1.1	16
16	Enhancing Ferromagnetism and Tuning Electronic Properties of CrI₃ Monolayers by Adsorption of Transition-Metal Atoms. ACS Applied Materials & Interfaces, 2021, 13, 21593-21601.	4.0	30
17	Atomistic Simulations of Defect Production in Monolayer and Bulk Hexagonal Boron Nitride under Low- and High-Fluence Ion Irradiation. Nanomaterials, 2021, 11, 1214.	1.9	7
18	Defect Agglomeration and Electron-Beam-Induced Local-Phase Transformations in Single-Layer MoTe₂. Journal of Physical Chemistry C, 2021, 125, 13601-13609.	1.5	14

#	Article	IF	Citations
19	Enhanced Trion Emission in Monolayer MoSe₂ by Constructing a Typeâ€Ⅱ Van Der Waals Heterostructure. Advanced Functional Materials, 2021, 31, 2104960.	7.8	21
20	Layer-Dependent Band Gaps of Platinum Dichalcogenides. ACS Nano, 2021, 15, 13249-13259.	7.3	41
21	Tunable electronic properties and enhanced ferromagnetism in Cr₂Ge₂Te₆ monolayer by strain engineering. Nanotechnology, 2021, 32, 485408.	1.3	7
22	Chlorine doping of MoSe₂ flakes by ion implantation. Nanoscale, 2021, 13, 5834-5846.	2.8	21
23	Water dissociation and association on mirror twin boundaries in two-dimensional MoSe₂: insights from density functional theory calculations. Nanoscale Advances, 2021, 3, 6992-7001.	2.2	4
24	Polymorphic Phases of Metal Chlorides in the Confined 2D Space of Bilayer Graphene. Advanced Materials, 2021, 33, e2105898.	11.1	12
25	Quasi-two-dimensional NaCl crystals encapsulated between graphene sheets and their decomposition under an electron beam. Nanoscale, 2021, 13, 19626-19633.	2.8	6
26	Gas Permeability and Selectivity of a Porous WS₂ Monolayer. Journal of Physical Chemistry C, 2021, 125, 25055-25066.	1.5	11
27	Boosting the Electrocatalytic Conversion of Nitrogen to Ammonia on Metal-Phthalocyanine-Based Two-Dimensional Conjugated Covalent Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 19992-20000.	6.6	100
28	Polymorphic Phases of Metal Chlorides in the Confined 2D Space of Bilayer Graphene (Adv. Mater.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	11.1	2
29	Channeling effects in gold nanoclusters under He ion irradiation: insights from molecular dynamics simulations. Nanotechnology, 2020, 31, 035302.	1.3	11
30	Reversible crystalline-to-amorphous phase transformation in monolayer MoS2 under grazing ion irradiation. 2D Materials, 2020, 7, 025005.	2.0	17
31	Tailoring the Electronic and Magnetic Properties of Hematene by Surface Passivation: Insights from First-Principles Calculations. Journal of Physical Chemistry C, 2020, 124, 22784-22792.	1.5	12
32	Freestanding and Supported MoS₂ Monolayers under Cluster Irradiation: Insights from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2020, 12, 37454-37463.	4.0	16
33	Are two-dimensional materials radiation tolerant?. Nanoscale Horizons, 2020, 5, 1447-1452.	4.1	26
34	Electron-beam-stimulated Atomic Migration Processes in Single-layer MoTe2. Microscopy and Microanalysis, 2020, 26, 534-537.	0.2	0
35	Electron Irradiation of Two-dimensional MoS2: Insights into the Influence of Electronic Excitations from First-principle Calculations. Microscopy and Microanalysis, 2020, 26, 784-785.	0.2	1
36	Strain robust spin gapless semiconductors/half-metals in transition metal embedded MoSe₂ monolayer. Journal of Physics Condensed Matter, 2020, 32, 365305.	0.7	9

#	Article	IF	Citations
37	Alkali metals inside bi-layer graphene and MoS2: Insights from first-principles calculations. Nano Energy, 2020, 75, 104927.	8.2	30
38	Enhanced Ferromagnetism and Tunable Magnetism in Fe₃GeTe₂ Monolayer by Strain Engineering. ACS Applied Materials & Interfaces, 2020, 12, 26367-26373.	4.0	83
39	Simulating Raman spectra by combining first-principles and empirical potential approaches with application to defective MoS2. Npj Computational Materials, 2020, 6, .	3.5	27
40	Synergistic electroreduction of carbon dioxide to carbon monoxide on bimetallic layered conjugated metal-organic frameworks. Nature Communications, 2020, 11, 1409.	5.8	317
41	Formation of Defects in Two-Dimensional MoS₂ in the Transmission Electron Microscope at Electron Energies below the Knock-on Threshold: The Role of Electronic Excitations. Nano Letters, 2020, 20, 2865-2870.	4.5	64
42	Revealing the defect-dominated oxygen evolution activity of hematene. Journal of Materials Chemistry A, 2020, 8, 6709-6716.	5.2	54
43	Band Bending and Valence Band Quantization at Line Defects in MoS₂. ACS Nano, 2020, 14, 9176-9187.	7.3	26
44	Local vibrational modes of Si vacancy spin qubits in SiC. Physical Review B, 2020, 101, .	1.1	25
45	Megacity Aerosol Pollution and Atmospheric Electric Field Disturbances. Izvestiya - Atmospheric and Oceanic Physics, 2020, 56, 759-772.	0.2	2
46	Enhanced sensitivity of MoSe₂ monolayer for gas adsorption induced by electric field. Journal of Physics Condensed Matter, 2019, 31, 445301.	0.7	35
47	Layer Rotation-Angle-Dependent Excitonic Absorption in van der Waals Heterostructures Revealed by Electron Energy Loss Spectroscopy. ACS Nano, 2019, 13, 9541-9550.	7.3	25
48	Nonstoichiometric Phases of Two-Dimensional Transition-Metal Dichalcogenides: From Chalcogen Vacancies to Pure Metal Membranes. Journal of Physical Chemistry Letters, 2019, 10, 6492-6498.	2.1	15
49	Which Transition Metal Atoms Can Be Embedded into Two-Dimensional Molybdenum Dichalcogenides and Add Magnetism?. Nano Letters, 2019, 19, 4581-4587.	4.5	61
50	Widely tunable GaAs bandgap via strain engineering in core/shell nanowires with large lattice mismatch. Nature Communications, 2019, 10, 2793.	5.8	78
51	Electron-Beam-Driven Structure Evolution of Single-Layer MoTe₂ for Quantum Devices. ACS Applied Nano Materials, 2019, 2, 3262-3270.	2.4	39
52	Tomonaga-Luttinger Liquid in a Box: Electrons Confined within <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ Mirror-Twin Boundaries. Physical Review X, 2019, 9, .	2.8	32
53	Roomâ€Temperature Ferromagnetism in MoTe₂ by Postâ€Growth Incorporation of Vanadium Impurities. Advanced Electronic Materials, 2019, 5, 1900044.	2.6	60
54	Thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml from molecular dynamics using different empirical potentials. Physical Review B, 2019, 99, .	1.1	50

#	Article	IF	Citations
55	Perforating Freestanding Molybdenum Disulfide Monolayers with Highly Charged Ions. Journal of Physical Chemistry Letters, 2019, 10, 904-910.	2.1	42
56	Effects of electron beam generated lattice defects on the periodic lattice distortion structure in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext>â^'</mml:mtext><mml:mm	1.1	7
57	Efficient method for calculating Raman spectra of solids with impurities and alloys and its application to two-dimensional transition metal dichalcogenides. Physical Review Materials, 2019, 3, .	0.9	17
58	Metallic Twin Boundaries Boost the Hydrogen Evolution Reaction on the Basal Plane of Molybdenum Selenotellurides. Advanced Energy Materials, 2018, 8, 1800031.	10.2	80
59	Post-Synthesis Modifications of Two-Dimensional MoSe₂ or MoTe₂ by Incorporation of Excess Metal Atoms into the Crystal Structure. ACS Nano, 2018, 12, 3975-3984.	7.3	67
60	Hydrogen-assisted post-growth substitution of tellurium into molybdenum disulfide monolayers with tunable compositions. Nanotechnology, 2018, 29, 145603.	1.3	17
61	MoS₂ Quantum Dots as Efficient Catalyst Materials for the Oxygen Evolution Reaction. ACS Catalysis, 2018, 8, 1683-1689.	5.5	215
62	Revealing the Atomic Defects of WS₂ Governing Its Distinct Optical Emissions. Advanced Functional Materials, 2018, 28, 1704210.	7.8	69
63	Reversible superdense ordering of lithium between two graphene sheets. Nature, 2018, 564, 234-239.	13.7	178
64	Observation of charge density waves in free-standing 1T-TaSe2 monolayers by transmission electron microscopy. Applied Physics Letters, 2018, 113, .	1.5	24
65	Electron Irradiation-Induced Defects and Phase Transformations in Two-Dimensional Transition Metal Dichalcogenides. Microscopy and Microanalysis, 2018, 24, 1592-1593.	0.2	1
66	1T phase as an efficient hole injection layer to TMDs transistors: a universal approach to achieve p-type contacts. 2D Materials, 2018, 5, 031012.	2.0	27
67	Nanostructuring few-layer graphene films with swift heavy ions for electronic application: tuning of electronic and transport properties. Nanoscale, 2018, 10, 14499-14509.	2.8	39
68	Advances in nanocarbon composite materials. Beilstein Journal of Nanotechnology, 2018, 9, 20-21.	1.5	10
69	Supported Two-Dimensional Materials under Ion Irradiation: The Substrate Governs Defect Production. ACS Applied Materials & Interfaces, 2018, 10, 30827-30836.	4.0	76
70	When defects are not defects. Nature Materials, 2018, 17, 757-758.	13.3	21
71	Atomic Defects and Doping of Monolayer NbSe₂. ACS Nano, 2017, 11, 2894-2904.	7.3	63
72	From Permeation to Cluster Arrays: Graphene on Ir(111) Exposed to Carbon Vapor. Nano Letters, 2017, 17, 3105-3112.	4.5	20

#	Article	IF	Citations
73	Two-dimensional MoS₂ under ion irradiation: from controlled defect production to electronic structure engineering. 2D Materials, 2017, 4, 025078.	2.0	146
74	Structural Transformations in Two-Dimensional Transition-Metal Dichalcogenide MoS₂ under an Electron Beam: Insights from First-Principles Calculations. Journal of Physical Chemistry Letters, 2017, 8, 3061-3067.	2.1	81
75	Acoustic gravity waves and the atmospheric electric field perturbations accompanying them. Geomagnetism and Aeronomy, 2017, 57, 335-346.	0.2	6
76	Revisiting Hollandites: Channels Filling by Main-Group Elements Together with Transition Metals in Bi2â€“yVyV8O16. Chemistry of Materials, 2017, 29, 5558-5565.	3.2	4
77	Tailoring the optical properties of atomically-thin WS₂via ion irradiation. Nanoscale, 2017, 9, 11027-11034.	2.8	84
78	Structural Distortions and Charge Density Waves in Iodine Chains Encapsulated inside Carbon Nanotubes. Nano Letters, 2017, 17, 3694-3700.	4.5	44
79	Engineering the Electronic Properties of Twoâ€Dimensional Transition Metal Dichalcogenides by Introducing Mirror Twin Boundaries. Advanced Electronic Materials, 2017, 3, 1600468.	2.6	85
80	Creating nanoporous graphene with swift heavy ions. Carbon, 2017, 114, 511-518.	5.4	52
81	Charge equilibration times for slow highly charged ions in single layer graphene. Journal of Physics: Conference Series, 2017, 875, 112001.	0.3	0
82	Engineering and modifying two-dimensional materials by electron beams. MRS Bulletin, 2017, 42, 667-676.	1.7	62
83	Interatomic Coulombic Decay: The Mechanism for Rapid Deexcitation of Hollow Atoms. Physical Review Letters, 2017, 119, 103401.	2.9	69
84	Substitutional carbon doping of free-standing and Ru-supported BN sheets: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 415301.	0.7	5
85	Luminescence of defects in the structural transformation of layered tin dichalcogenides. Applied Physics Letters, 2017, 111, .	1.5	16
86	Vibrational Properties of Metal Phosphorus Trichalcogenides from First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 27207-27217.	1.5	68
87	Towards diluted magnetism in TaAs. Physical Review Materials, 2017, 1, .	0.9	3
88	Tailoring Optical Properties of Atomically-Thin WS2 via Ion Irradiation. , 2017, , .		0
89	Ultrafast electronic response of graphene to a strong and localized electric field. Nature Communications, 2016, 7, 13948.	5.8	125
90	Study of acoustic emission signals during fracture shear deformation. Acoustical Physics, 2016, 62, 505-513.	0.2	17

#	Article	IF	Citations
91	Vibrational Properties of a Two-Dimensional Silica Kagome Lattice. ACS Nano, 2016, 10, 10929-10935.	7.3	18
92	Mechanical properties and current-carrying capacity of Al reinforced with graphene/BN nanoribbons: a computational study. Nanoscale, 2016, 8, 20080-20089.	2.8	19
93	Electron-Beam Induced Transformations of Layered Tin Dichalcogenides. Nano Letters, 2016, 16, 4410-4416.	4.5	109
94	Nanostructured BNâ€“Mg composites: features of interface bonding and mechanical properties. Physical Chemistry Chemical Physics, 2016, 18, 965-969.	1.3	12
95	Phosphorene under electron beam: from monolayer to one-dimensional chains. Nanoscale, 2016, 8, 7949-7957.	2.8	51
96	Native defects in bulk and monolayer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> first principles. Physical Review B, 2015, 91, .	1.1	438
97	Xe irradiation of graphene on Ir(111): From trapping to blistering. Physical Review B, 2015, 92, .	1.1	32
98	Silicon and silicon-nitrogen impurities in graphene: Structure, energetics, and effects on electronic transport. Physical Review B, 2015, 92, .	1.1	23
99	Simulations of electromechanical shape transformations of Au nanoparticles. Physica Status Solidi (B): Basic Research, 2015, 252, 144-148.	0.7	2
100	Atomic scale interface design and characterisation. Beilstein Journal of Nanotechnology, 2015, 6, 1708-1711.	1.5	2
101	Simulations of electromechanical shape transformations of Au nanoparticles (Phys. Status Solidi B) Tj ETQq1 1 0.784314 rgBT /Overlock	0.7	0
102	Atomic Scale Microstructure and Properties of Se-Deficient Two-Dimensional MoSe₂. ACS Nano, 2015, 9, 3274-3283.	7.3	213
103	Solubility of Boron, Carbon, and Nitrogen in Transition Metals: Getting Insight into Trends from First-Principles Calculations. Journal of Physical Chemistry Letters, 2015, 6, 3263-3268.	2.1	50
104	Comment on â€œInterfacial Carbon Nanoplatelet Formation by Ion Irradiation of Graphene on Iridium(111)â€• ACS Nano, 2015, 9, 4664-4665.	7.3	10
105	Line and rotational defects in boron-nitrene: Structure, energetics, and dependence on mechanical strain from first-principles calculations. Physica Status Solidi (B): Basic Research, 2015, 252, 1725-1730.	0.7	7
106	Three-fold rotational defects in two-dimensional transition metal dichalcogenides. Nature Communications, 2015, 6, 6736.	5.8	179
107	Single-Layer ReS₂: Two-Dimensional Semiconductor with Tunable In-Plane Anisotropy. ACS Nano, 2015, 9, 11249-11257.	7.3	353
108	Interfacial Carbon Nanoplatelet Formation by Ion Irradiation of Graphene on Iridium(111). ACS Nano, 2014, 8, 12208-12218.	7.3	29

#	Article	IF	Citations
109	Experimental Observation of Boron Nitride Chains. ACS Nano, 2014, 8, 11950-11957.	7.3	70
110	Charged Point Defects in the Flatland: Accurate Formation Energy Calculations in Two-Dimensional Materials. Physical Review X, 2014, 4, .	2.8	67
111	Frontispiece: Triazine-Based Graphitic Carbon Nitride: a Two-Dimensional Semiconductor. Angewandte Chemie - International Edition, 2014, 53, n/a-n/a.	7.2	0
112	Frontispiz: Triazine-Based Graphitic Carbon Nitride: a Two-Dimensional Semiconductor. Angewandte Chemie, 2014, 126, n/a-n/a.	1.6	0
113	Properties of Individual Dopant Atoms in Singleâ€Layer MoS₂: Atomic Structure, Migration, and Enhanced Reactivity. Advanced Materials, 2014, 26, 2857-2861.	11.1	258
114	Triazineâ€Based Graphitic Carbon Nitride: a Twoâ€Dimensional Semiconductor. Angewandte Chemie - International Edition, 2014, 53, 7450-7455.	7.2	523
115	Electronic stopping power from first-principles calculations with account for core electron excitations and projectile ionization. Physical Review B, 2014, 89, .	1.1	89
116	Toward Stronger Alâ€“BN Nanotube Composite Materials: Insights into Bonding at the Al/BN Interface from First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 26894-26901.	1.5	24
117	Solid-State Growth of One- and Two-Dimensional Silica Structures on Metal Surfaces. Journal of Physical Chemistry C, 2014, 118, 21001-21005.	1.5	7
118	Semiconductor to Metal to Half-Metal Transition in Pt-Embedded Zigzag Graphene Nanoribbons. Journal of Physical Chemistry C, 2014, 118, 16133-16139.	1.5	22
119	Atomic structure and dynamic behaviour of trulyÂone-dimensional ionic chains inside carbonÂnanotubes. Nature Materials, 2014, 13, 1050-1054.	13.3	82
120	Coronene Encapsulation in Singleâ€Walled Carbon Nanotubes: Stacked Columns, Peapods, and Nanoribbons. ChemPhysChem, 2014, 15, 1660-1665.	1.0	28
121	Fabrication and atomic structure of size-selected, layered MoS₂clusters for catalysis. Nanoscale, 2014, 6, 12463-12469.	2.8	37
122	Doping Properties and Phase Transition in Single-Layer MoS2. Microscopy and Microanalysis, 2014, 20, 1750-1751.	0.2	1
123	Inorganic Two-Dimensional Materials under Electron Irradiation: Stability, Evolution of the Atomic Structure, and Beam-Mediated Doping. Microscopy and Microanalysis, 2014, 20, 1756-1757.	0.2	0
124	Atomic scale study of the life cycle of a dislocation in graphene from birth to annihilation. Nature Communications, 2013, 4, 2098.	5.8	149
125	Strains Induced by Point Defects in Graphene on a Metal. Physical Review Letters, 2013, 111, 085501.	2.9	51
126	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. Physical Review B, 2013, 87, .	1.1	162

#	Article	IF	Citations
127	Electronic structures and optical properties of realistic transition metal dichalcogenide heterostructures from first principles. Physical Review B, 2013, 88, .	1.1	400
128	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. Scientific Reports, 2013, 3, 3482.	1.6	80
129	From point to extended defects in two-dimensional MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: Evolution of atomic structure under electron irradiation. Physical Review B, 2013, 88, .	1.1	408
130	Ionâ€Irradiationâ€Induced Defects in Isotopicallyâ€Labeled Two Layered Graphene: Enhanced Inâ€Situ Annealing of the Damage. Advanced Materials, 2013, 25, 1004-1009.	11.1	79
131	Doped Graphene as a Material for Oxygen Reduction Reaction in Hydrogen Fuel Cells: A Computational Study. ACS Catalysis, 2013, 3, 159-165.	5.5	100
132	Chiralityâ€Dependent Reactivity of Individual Singleâ€Walled Carbon Nanotubes. Small, 2013, 9, 1379-1386.	5.2	41
133	Ion Impacts on Graphene/Ir(111): Interface Channeling, Vacancy Funnels, and a Nanomesh. Nano Letters, 2013, 13, 1948-1955.	4.5	81
134	Dual origin of defect magnetism in graphene and its reversible switching by molecular doping. Nature Communications, 2013, 4, 2010.	5.8	230
135	In Situ Growth of Cellular Two-Dimensional Silicon Oxide on Metal Substrates. ACS Nano, 2013, 7, 5175-5180.	7.3	31
136	Ion irradiation tolerance of graphene as studied by atomistic simulations. Applied Physics Letters, 2012, 100, 233108.	1.5	42
137	Tuning electronic and magnetic properties of zigzag graphene nanoribbons by large-scale bending. Applied Physics Letters, 2012, 100, .	1.5	14
138	Two-Dimensional Transition Metal Dichalcogenide Alloys: Stability and Electronic Properties. Journal of Physical Chemistry Letters, 2012, 3, 3652-3656.	2.1	290
139	Atomistic Description of Electron Beam Damage in Nitrogen-Doped Graphene and Single-Walled Carbon Nanotubes. ACS Nano, 2012, 6, 8837-8846.	7.3	119
140	Effects of confinement and environment on the electronic structure and exciton binding energy of MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2012, 86, .	1.1	539
141	The Role of Stable and Mobile Carbon Adspecies in Copper-Promoted Graphene Growth. Journal of Physical Chemistry C, 2012, 116, 5802-5809.	1.5	70
142	Two-Dimensional Transition Metal Dichalcogenides under Electron Irradiation: Defect Production and Doping. Physical Review Letters, 2012, 109, 035503.	2.9	960
143	Accurate Measurement of Electron Beam Induced Displacement Cross Sections for Single-Layer Graphene. Physical Review Letters, 2012, 108, 196102.	2.9	383
144	Are we van der Waals ready?. Journal of Physics Condensed Matter, 2012, 24, 424218.	0.7	129

#	Article	IF	Citations
145	Stability of Graphene Edges under Electron Beam: Equilibrium Energetics versus Dynamic Effects. ACS Nano, 2012, 6, 671-676.	7.3	120
146	Gold-embedded zigzag graphene nanoribbons as spin gapless semiconductors. Physical Review B, 2012, 86, .	1.1	48
147	Spin-half paramagnetism in graphene induced by point defects. Nature Physics, 2012, 8, 199-202.	6.5	743
148	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. Physical Review Letters, 2012, 108, 235502.	2.9	851
149	Direct Imaging of a Two-Dimensional Silica Glass on Graphene. Nano Letters, 2012, 12, 1081-1086.	4.5	236
150	Engineering the Atomic Structure of Carbon Nanotubes by a Focused Electron Beam: New Morphologies at the Subâ€Nanometer Scale. ChemPhysChem, 2012, 13, 2596-2600.	1.0	19
151	Atom-by-Atom Observation of Grain Boundary Migration in Graphene. Nano Letters, 2012, 12, 3168-3173.	4.5	178
152	Atomistic simulations of the implantation of low-energy boron and nitrogen ions into graphene. Physical Review B, 2011, 83, .	1.1	127
153	Characterization of ion-irradiation-induced defects in multi-walled carbon nanotubes. New Journal of Physics, 2011, 13, 073004.	1.2	55
154	Cutting and controlled modification of graphene with ion beams. Nanotechnology, 2011, 22, 175306.	1.3	130
155	From Point Defects in Graphene to Two-Dimensional Amorphous Carbon. Physical Review Letters, 2011, 106, 105505.	2.9	675
156	Structural Defects in Graphene. ACS Nano, 2011, 5, 26-41.	7.3	2,818
157	Stone-Wales-type transformations in carbon nanostructures driven by electron irradiation. Physical Review B, 2011, 83, .	1.1	226
158	Synthesis of Graphene Nanoribbons Encapsulated in Single-Walled Carbon Nanotubes. Nano Letters, 2011, 11, 4352-4356.	4.5	174
159	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. Physical Review B, 2011, 84, .	1.1	32
160	Attractive interaction between transition-metal atom impurities and vacancies in graphene: a first-principles study. Theoretical Chemistry Accounts, 2011, 129, 625-630.	0.5	97
161	Production of defects in hexagonal boron nitride monolayer under ion irradiation. Nuclear Instruments & Methods in Physics Research B, 2011, 269, 1327-1331.	0.6	50
162	Mechanism of swift chemical sputtering: Comparison of Be/C/W dimer bond breaking. Nuclear Instruments & Methods in Physics Research B, 2011, 269, 1257-1261.	0.6	12

#	Article	IF	Citations
163	Berseneva, Krasheninnikov, and Nieminen Reply:. Physical Review Letters, 2011, 107, .	2.9	6
164	Mechanisms of Postsynthesis Doping of Boron Nitride Nanostructures with Carbon from First-Principles Simulations. Physical Review Letters, 2011, 107, 035501.	2.9	88
165	Submonolayers of carbon on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>-Fe</mml:mtext></mml:mrow></mml:math>facets: Anab initiostudy. Physical Review B, 2010, 82, .	1.1	17
166	Ion and electron irradiation-induced effects in nanostructured materials. Journal of Applied Physics, 2010, 107, .	1.1	878
167	Ion irradiation of multiâ€walled boron nitride nanotubes. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, 1256-1259.	0.8	17
168	Boron nitride formation on magnesium studied byab initiocalculations. Physical Review B, 2010, 81, .	1.1	5
169	Response of mechanically strained nanomaterials to irradiation: Insight from atomistic simulations. Physical Review B, 2010, 82, .	1.1	26
170	Effects of ion bombardment on a two-dimensional target: Atomistic simulations of graphene irradiation. Physical Review B, 2010, 81, .	1.1	341
171	A first-principles study on magnetic coupling between carbon adatoms on graphene. New Journal of Physics, 2010, 12, 113021.	1.2	30
172	Migration of gold atoms in graphene ribbons: Role of the edges. Physical Review B, 2010, 81, .	1.1	41
173	Effect of iron nanoparticle geometry on the energetics of carbon interstititals. Physica Status Solidi C: Current Topics in Solid State Physics, 2010, 7, NA-NA.	0.8	3
174	Defect-induced junctions between single- or double-wall carbon nanotubes and metal crystals. Nanoscale, 2010, 2, 901.	2.8	19
175	Migration and Localization of Metal Atoms on Strained Graphene. Physical Review Letters, 2010, 105, 196102.	2.9	304
176	Electron knock-on damage in hexagonal boron nitride monolayers. Physical Review B, 2010, 82, .	1.1	241
177	Modifying the electronic structure of semiconducting single-walled carbon nanotubes byAr+ion irradiation. Physical Review B, 2009, 79, .	1.1	42
178	Computational study of boron nitride nanotube synthesis: How catalyst morphology stabilizes the boron nitride bond. Physical Review B, 2009, 80, .	1.1	16
179	Quantum and Classical Molecular Dynamics Studies of the Threshold Displacement Energy in Si Bulk and Nanowires. Materials Research Society Symposia Proceedings, 2009, 1181, 72.	0.1	4
180	Growth of Singleâ€Walled Carbon Nanotubes from Sharp Metal Tips. Small, 2009, 5, 2710-2715.	5.2	29

#	Article	IF	Citations
181	Embedding Transition-Metal Atoms in Graphene: Structure, Bonding, and Magnetism. Physical Review Letters, 2009, 102, 126807.	2.9	1,022
182	Effects of ion beam heating on Raman spectra of single-walled carbon nanotubes. Applied Physics Letters, 2009, 94, .	1.5	8
183	Electrical properties of C⁴⁺ irradiated singleâ€walled carbon nanotube paper. Physica Status Solidi (B): Basic Research, 2008, 245, 2280-2283.	0.7	21
184	Ion irradiation of carbon nanotubes encapsulating cobalt crystals. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 2618-2621.	1.3	11
185	The diffusion of carbon atoms inside carbon nanotubes. New Journal of Physics, 2008, 10, 023022.	1.2	42
186	Plastic Deformation of Single Nanometer-Sized Crystals. Physical Review Letters, 2008, 101, 156101.	2.9	70
187	Atomistic Computer Simulations of Irradiation-Induced Effects in Nanostructured Carbon Materials. Journal of Computational and Theoretical Nanoscience, 2008, 5, 1828-1851.	0.4	11
188	In-situ electron irradiation studies of metal-carbon nanostructures. , 2008, , 121-122.		0
189	Comment on â€œPaired Gap States in a Semiconducting Carbon Nanotube: Deep and Shallow Levelsâ€• Physical Review Letters, 2007, 99, 179703; author reply 179704.	2.9	3
190	Relative abundance of single and double vacancies in irradiated single-walled carbon nanotubes. Applied Physics Letters, 2007, 91, 173109.	1.5	45
191	Role of Electronic Excitations in Ion Collisions with Carbon Nanostructures. Physical Review Letters, 2007, 99, 016104.	2.9	142
192	Atomistic simulations of irradiation effects in carbon nanotubes: an overview. Radiation Effects and Defects in Solids, 2007, 162, 157-169.	0.4	17
193	Engineering of nanostructured carbon materials with electron or ion beams. Nature Materials, 2007, 6, 723-733.	13.3	898
194	A novel hybrid carbon material. Nature Nanotechnology, 2007, 2, 156-161.	15.6	369
195	Creation of paired electron states in the gap of semiconducting carbon nanotubes by correlated hydrogen adsorption. New Journal of Physics, 2007, 9, 275-275.	1.2	33
196	Kinetic Monte Carlo Simulations of the Response of Carbon Nanotubes to Electron Irradiation. Journal of Computational and Theoretical Nanoscience, 2007, 4, 1153-1159.	0.4	19
197	Carbon Nanotubes as High-Pressure Cylinders and Nanoextruders. Science, 2006, 312, 1199-1202.	6.0	283
198	Energetics, structure, and long-range interaction of vacancy-type defects in carbon nanotubes: Atomistic simulations. Physical Review B, 2006, 74, .	1.1	202

#	Article	IF	Citations
199	Nitrogen-doped carbon nanotubes under electron irradiation simulated with a tight-binding model. Physical Review B, 2006, 74, .	1.1	17
200	Swift chemical sputtering of covalently bonded materials. Pure and Applied Chemistry, 2006, 78, 1203-1211.	0.9	26
201	Bending the rules: Contrasting vacancy energetics and migration in graphite and carbon nanotubes. Chemical Physics Letters, 2006, 418, 132-136.	1.2	302
202	Channeling of heavy ions through multi-walled carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 21-25.	0.6	29
203	A molecular dynamics study of the clustering of implanted potassium in multiwalled carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2005, 240, 810-818.	0.6	14
204	Irradiation-assisted substitution of carbon atoms with nitrogen and boron in single-walled carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 31-36.	0.6	29
205	Irradiation-induced stiffening of carbon nanotube bundles. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 142-145.	0.6	49
206	Difference in formation of hydrogen and helium clusters in tungsten. Applied Physics Letters, 2005, 87, 163113.	1.5	145
207	B and N ion implantation into carbon nanotubes: Insight from atomistic simulations. Physical Review B, 2005, 71, .	1.1	88
208	Carbon nanotubes under electron irradiation: Stability of the tubes and their action as pipes for atom transport. Physical Review B, 2005, 71, .	1.1	121
209	Stability of carbon nanotubes under electron irradiation: Role of tube diameter and chirality. Physical Review B, 2005, 72, .	1.1	146
210	Multiwalled carbon nanotubes as apertures and conduits for energetic ions. Physical Review B, 2005, 71, .	1.1	47
211	Nitrogen in graphite and carbon nanotubes: Magnetism and mobility. Physical Review B, 2005, 72, .	1.1	117
212	Structure and stability of non-molecular nitrogen at ambient pressure. Europhysics Letters, 2004, 65, 400-406.	0.7	20
213	Carbon Nanotube Mats and Fibers with Irradiation-Improved Mechanical Characteristics: A Theoretical Model. Physical Review Letters, 2004, 93, 215503.	2.9	64
214	Improved mechanical load transfer between shells of multiwalled carbon nanotubes. Physical Review B, 2004, 70, .	1.1	141
215	Irradiation effects in carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2004, 216, 355-366.	0.6	204
216	Adsorption and migration of carbon adatoms on carbon nanotubes: Density-functionalab initioand tight-binding studies. Physical Review B, 2004, 69, .	1.1	111

#	Article	IF	Citations
217	Mechanical properties of carbon nanotubes with vacancies and related defects. Physical Review B, 2004, 70, .	1.1	349
218	Adsorption and migration of carbon adatoms on zigzag carbon nanotubes. Carbon, 2004, 42, 1021-1025.	5.4	52
219	Irradiation-Induced Magnetism in Graphite: A Density Functional Study. Physical Review Letters, 2004, 93, 187202.	2.9	612
220	Ion ranges and irradiation-induced defects in multiwalled carbon nanotubes. Journal of Applied Physics, 2004, 96, 2864-2871.	1.1	88
221	Making junctions between carbon nanotubes using an ion beam. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 224-229.	0.6	27
222	Stopping of energetic ions in carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2003, 206, 18-21.	0.6	28
223	Molecular dynamics simulations of CH3 sticking on carbon first wall structures. Journal of Nuclear Materials, 2003, 313-316, 52-55.	1.3	12
224	Magnetic Properties and Diffusion of Adatoms on a Graphene Sheet. Physical Review Letters, 2003, 91, 017202.	2.9	419
225	Atomic-scale simulations of radiation effects in GaN and carbon nanotubes. Materials Research Society Symposia Proceedings, 2003, 792, 440.	0.1	0
226	Molecular dynamics simulations of CH3 sticking on carbon surfaces. Journal of Applied Physics, 2003, 93, 1826-1831.	1.1	18
227	Carbon nanotubes as masks against ion irradiation: An insight from atomistic simulations. Applied Physics Letters, 2002, 81, 1101-1103.	1.5	37
228	Stability of irradiation-induced point defects on walls of carbon nanotubes. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 2002, 20, 728.	1.6	57
229	Ion-irradiation-induced welding of carbon nanotubes. Physical Review B, 2002, 66, .	1.1	144
230	Sputtering of amorphous hydrogenated carbon by hyperthermal ions as studied by tight-binding molecular dynamics. Computational Materials Science, 2002, 25, 427-434.	1.4	29
231	Production of defects in supported carbon nanotubes under ion irradiation. Physical Review B, 2002, 65, .	1.1	203
232	Ion-irradiation-induced defects in bundles of carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2002, 193, 603-608.	0.6	91
233	Tight-Binding Atomistic Simulations of Hydrocarbon Sputtering by Hyperthermal Ions in Tokamak Divertors. Contributions To Plasma Physics, 2002, 42, 451-457.	0.5	7
234	Signatures of irradiation-induced defects in scanning-tunneling microscopy images of carbon nanotubes. Physics of the Solid State, 2002, 44, 470-472.	0.2	12

#	Article	IF	Citations
235	Formation of ion-irradiation-induced atomic-scale defects on walls of carbon nanotubes. Physical Review B, 2001, 63, .	1.1	294
236	Effects of Ion Irradiation on Supported Carbon Nanotubes and Nanotube-Substrate Interfaces. Materials Research Society Symposia Proceedings, 2001, 706, 1.	0.1	0
237	Predicted scanning tunneling microscopy images of carbon nanotubes with atomic vacancies. Solid State Communications, 2001, 118, 361-365.	0.9	36
238	The effect of interstitial clusters and vacancies on the scanning tunneling microscopy image of graphite. Surface Science, 2000, 454-456, 519-524.	0.8	26
239	Kinetic theory of cascade laser based on quantum wells and wires. Physica A: Statistical Mechanics and Its Applications, 1997, 241, 386-392.	1.2	1
240	Kinetic theory of semiconductor cascade laser based on quantum wells and wires. Journal of Experimental and Theoretical Physics, 1997, 84, 375-382.	0.2	3
241	Generation of one-photon states by a quantum dot. Journal of Experimental and Theoretical Physics, 1997, 85, 682-689.	0.2	3
242	Elementary quantum-dot gates for single-electron computing. JETP Letters, 1996, 64, 231-236.	0.4	7
243	Is the gap anisotropy in high-Tc superconductors really as high as it is commonly believed?. Physica C: Superconductivity and Its Applications, 1996, 257, 53-60.	0.6	8
244	Pairing correlations withs*anddx2â^'y2symmetry in a disorderedCu4O8cluster. Physical Review B, 1995, 52, 16187-16191.	1.1	0
245	Metal-insulator transition in Emery-Anderson model. Density of states calculations. Physica C: Superconductivity and Its Applications, 1994, 222, 127-132.	0.6	4
246	Extrinsic Localized Excitons in Patterned 2D Semiconductors. Advanced Functional Materials, 0, , 2203060.	7.8	8