Arkady Krasheninnikov

List of Publications by Year
in descending order

246 papers	26,941 citations	8732 75 h-index	5965 160 g-index
259 all docs	259 docs citations	259 times ranked	24237 citing authors

#	Article	IF	Citations
1	Structural Defects in Graphene. ACS Nano, 2011, 5, 26-41.	7.3	2,818
2	Embedding Transition-Metal Atoms in Graphene: Structure, Bonding, and Magnetism. Physical Review Letters, 2009, 102, 126807.	2.9	1,022
3	Two-Dimensional Transition Metal Dichalcogenides under Electron Irradiation: Defect Production and Doping. Physical Review Letters, 2012, 109, 035503.	2.9	960
4	Engineering of nanostructured carbon materials with electron or ion beams. Nature Materials, 2007, 6, 723-733.	13.3	898
5	Ion and electron irradiation-induced effects in nanostructured materials. Journal of Applied Physics, 2010, 107, .	1.1	878
6	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. Physical Review Letters, 2012, 108, 235502.	2.9	851
7	Spin-half paramagnetism in graphene induced by point defects. Nature Physics, 2012, 8, 199-202.	6.5	743
8	From Point Defects in Graphene to Two-Dimensional Amorphous Carbon. Physical Review Letters, 2011, 106, 105505.	2.9	675
9	Irradiation-Induced Magnetism in Graphite: A Density Functional Study. Physical Review Letters, 2004, 93, 187202.	2.9	612
10	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
11	Triazineâ€Based Graphitic Carbon Nitride: a Twoâ€Dimensional Semiconductor. Angewandte Chemie - International Edition, 2014, 53, 7450-7455.	7.2	523
12	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></mn first principles. Physical Review B, 2015, 91, .	1.1	435
13	Magnetic Properties and Diffusion of Adatoms on a Graphene Sheet. Physical Review Letters, 2003, 91, 017202.	2.9	419
14	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
15	Electronic structures and optical properties of realistic transition metal dichalcogenide heterostructures from first principles. Physical Review B, 2013, 88, .	1.1	400
16	Accurate Measurement of Electron Beam Induced Displacement Cross Sections for Single-Layer Graphene. Physical Review Letters, 2012, 108, 196102.	2.9	383
17	A novel hybrid carbon material. Nature Nanotechnology, 2007, 2, 156-161.	15.6	369
18	Single-Layer ReS₂: Two-Dimensional Semiconductor with Tunable In-Plane Anisotropy. ACS Nano, 2015, 9, 11249-11257.	7.3	353

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19	Mechanical properties of carbon nanotubes with vacancies and related defects. Physical Review B, 2004, 70, .	1.1	349
20	Effects of ion bombardment on a two-dimensional target: Atomistic simulations of graphene irradiation. Physical Review B, 2010, 81, .	1.1	341
21	Synergistic electroreduction of carbon dioxide to carbon monoxide on bimetallic layered conjugated metal-organic frameworks. Nature Communications, 2020, 11, 1409.	5.8	317
22	Migration and Localization of Metal Atoms on Strained Graphene. Physical Review Letters, 2010, 105, 196102.	2.9	304
23	Bending the rules: Contrasting vacancy energetics and migration in graphite and carbon nanotubes. Chemical Physics Letters, 2006, 418, 132-136.	1.2	302
24	Formation of ion-irradiation-induced atomic-scale defects on walls of carbon nanotubes. Physical Review B, 2001, 63, .	1.1	294
25	Two-Dimensional Transition Metal Dichalcogenide Alloys: Stability and Electronic Properties. Journal of Physical Chemistry Letters, 2012, 3, 3652-3656.	2.1	290
26	Carbon Nanotubes as High-Pressure Cylinders and Nanoextruders. Science, 2006, 312, 1199-1202.	6.0	283
27	Properties of Individual Dopant Atoms in Singleâ€Layer MoS₂: Atomic Structure, Migration, and Enhanced Reactivity. Advanced Materials, 2014, 26, 2857-2861.	11.1	258
28	Electron knock-on damage in hexagonal boron nitride monolayers. Physical Review B, 2010, 82, .	1.1	241
29	Direct Imaging of a Two-Dimensional Silica Glass on Graphene. Nano Letters, 2012, 12, 1081-1086.	4.5	236
30	Dual origin of defect magnetism in graphene and its reversible switching by molecular doping. Nature Communications, 2013, 4, 2010.	5.8	230
31	Stone-Wales-type transformations in carbon nanostructures driven by electron irradiation. Physical Review B, 2011, 83, .	1.1	226
32	MoS₂ Quantum Dots as Efficient Catalyst Materials for the Oxygen Evolution Reaction. ACS Catalysis, 2018, 8, 1683-1689.	5.5	215
33	Atomic Scale Microstructure and Properties of Se-Deficient Two-Dimensional MoSe₂. ACS Nano, 2015, 9, 3274-3283.	7.3	213
34	Irradiation effects in carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2004, 216, 355-366.	0.6	204
35	Production of defects in supported carbon nanotubes under ion irradiation. Physical Review B, 2002, 65, .	1.1	203
36	Energetics, structure, and long-range interaction of vacancy-type defects in carbon nanotubes: Atomistic simulations. Physical Review B, 2006, 74, .	1.1	202

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37	Three-fold rotational defects in two-dimensional transition metal dichalcogenides. Nature Communications, 2015, 6, 6736.	5.8	179
38	Atom-by-Atom Observation of Grain Boundary Migration in Graphene. Nano Letters, 2012, 12, 3168-3173.	4.5	178
39	Reversible superdense ordering of lithium between two graphene sheets. Nature, 2018, 564, 234-239.	13.7	178
40	Synthesis of Graphene Nanoribbons Encapsulated in Single-Walled Carbon Nanotubes. Nano Letters, 2011, 11, 4352-4356.	4.5	174
41	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. Physical Review B, 2013, 87, .	1.1	162
42	Atomic scale study of the life cycle of a dislocation in graphene from birth to annihilation. Nature Communications, 2013, 4, 2098.	5.8	149
43	Stability of carbon nanotubes under electron irradiation: Role of tube diameter and chirality. Physical Review B, 2005, 72, .	1.1	146
44	Two-dimensional MoS₂ under ion irradiation: from controlled defect production to electronic structure engineering. 2D Materials, 2017, 4, 025078.	2.0	146
45	Difference in formation of hydrogen and helium clusters in tungsten. Applied Physics Letters, 2005, 87, 163113.	1.5	145
46	Ion-irradiation-induced welding of carbon nanotubes. Physical Review B, 2002, 66, .	1.1	144
47	Role of Electronic Excitations in Ion Collisions with Carbon Nanostructures. Physical Review Letters, 2007, 99, 016104.	2.9	142
48	Improved mechanical load transfer between shells of multiwalled carbon nanotubes. Physical Review B, 2004, 70, .	1.1	141
49	Cutting and controlled modification of graphene with ion beams. Nanotechnology, 2011, 22, 175306.	1.3	130
50	Are we van der Waals ready?. Journal of Physics Condensed Matter, 2012, 24, 424218.	0.7	129
51	Atomistic simulations of the implantation of low-energy boron and nitrogen ions into graphene. Physical Review B, 2011, 83, .	1.1	127
52	Ultrafast electronic response of graphene to a strong and localized electric field. Nature Communications, 2016, 7, 13948.	5.8	125
53	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
54	Stability of Graphene Edges under Electron Beam: Equilibrium Energetics <i>versus</i> Dynamic Effects. ACS Nano, 2012, 6, 671-676.	7.3	120

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55	Atomistic Description of Electron Beam Damage in Nitrogen-Doped Graphene and Single-Walled Carbon Nanotubes. ACS Nano, 2012, 6, 8837-8846.	7.3	119
56	Nitrogen in graphite and carbon nanotubes: Magnetism and mobility. Physical Review B, 2005, 72, .	1.1	117
57	Adsorption and migration of carbon adatoms on carbon nanotubes: Density-functionalab initioand tight-binding studies. Physical Review B, 2004, 69, .	1.1	111
58	Electron-Beam Induced Transformations of Layered Tin Dichalcogenides. Nano Letters, 2016, 16, 4410-4416.	4.5	109
59	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
60	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
61	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
62	Ion-irradiation-induced defects in bundles of carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2002, 193, 603-608.	0.6	91
63	Electronic stopping power from first-principles calculations with account for core electron excitations and projectile ionization. Physical Review B, 2014, 89, .	1.1	89
64	Ion ranges and irradiation-induced defects in multiwalled carbon nanotubes. Journal of Applied Physics, 2004, 96, 2864-2871.	1.1	88
65	B and N ion implantation into carbon nanotubes: Insight from atomistic simulations. Physical Review B, 2005, 71, .	1.1	88
66	Mechanisms of Postsynthesis Doping of Boron Nitride Nanostructures with Carbon from First-Principles Simulations. Physical Review Letters, 2011, 107, 035501.	2.9	88
67	Engineering the Electronic Properties of Twoâ€Dimensional Transition Metal Dichalcogenides by Introducing Mirror Twin Boundaries. Advanced Electronic Materials, 2017, 3, 1600468.	2.6	85
68	Tailoring the optical properties of atomically-thin WS₂via ion irradiation. Nanoscale, 2017, 9, 11027-11034.	2.8	84
69	Enhanced Ferromagnetism and Tunable Magnetism in Fe₃GeTe₂ Monolayer by Strain Engineering. ACS Applied Materials & Interfaces, 2020, 12, 26367-26373.	4.0	83
70	Atomic structure and dynamic behaviour of trulyÂone-dimensional ionic chains inside carbonÂnanotubes. Nature Materials, 2014, 13, 1050-1054.	13.3	82
71	Ion Impacts on Graphene/Ir(111): Interface Channeling, Vacancy Funnels, and a Nanomesh. Nano Letters, 2013, 13, 1948-1955.	4.5	81
72	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

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73	Defects in bilayer silica and graphene: common trends in diverse hexagonal two-dimensional systems. Scientific Reports, 2013, 3, 3482.	1.6	80
74	Metallic Twin Boundaries Boost the Hydrogen Evolution Reaction on the Basal Plane of Molybdenum Selenotellurides. Advanced Energy Materials, 2018, 8, 1800031.	10.2	80
75	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
76	Widely tunable GaAs bandgap via strain engineering in core/shell nanowires with large lattice mismatch. Nature Communications, 2019, 10, 2793.	5.8	78
77	Supported Two-Dimensional Materials under Ion Irradiation: The Substrate Governs Defect Production. ACS Applied Materials & Interfaces, 2018, 10, 30827-30836.	4.0	76
78	Plastic Deformation of Single Nanometer-Sized Crystals. Physical Review Letters, 2008, 101, 156101.	2.9	70
79	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
80	Experimental Observation of Boron Nitride Chains. ACS Nano, 2014, 8, 11950-11957.	7.3	70
81	Interatomic Coulombic Decay: The Mechanism for Rapid Deexcitation of Hollow Atoms. Physical Review Letters, 2017, 119, 103401.	2.9	69
82	Revealing the Atomic Defects of WS₂ Governing Its Distinct Optical Emissions. Advanced Functional Materials, 2018, 28, 1704210.	7.8	69
83	Vibrational Properties of Metal Phosphorus Trichalcogenides from First-Principles Calculations. Journal of Physical Chemistry C, 2017, 121, 27207-27217.	1.5	68
84	Charged Point Defects in the Flatland: Accurate Formation Energy Calculations in Two-Dimensional Materials. Physical Review X, 2014, 4, .	2.8	67
85	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
86	Carbon Nanotube Mats and Fibers with Irradiation-Improved Mechanical Characteristics: A Theoretical Model. Physical Review Letters, 2004, 93, 215503.	2.9	64
87	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
88	Atomic Defects and Doping of Monolayer NbSe₂. ACS Nano, 2017, 11, 2894-2904.	7.3	63
89	Engineering and modifying two-dimensional materials by electron beams. MRS Bulletin, 2017, 42, 667-676.	1.7	62
90	Which Transition Metal Atoms Can Be Embedded into Two-Dimensional Molybdenum Dichalcogenides and Add Magnetism?. Nano Letters, 2019, 19, 4581-4587.	4.5	61

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91	Roomâ€Temperature Ferromagnetism in MoTe₂ by Postâ€Growth Incorporation of Vanadium Impurities. Advanced Electronic Materials, 2019, 5, 1900044.	2.6	60
92	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
93	Characterization of ion-irradiation-induced defects in multi-walled carbon nanotubes. New Journal of Physics, 2011, 13, 073004.	1.2	55
94	Revealing the defect-dominated oxygen evolution activity of hematene. Journal of Materials Chemistry A, 2020, 8, 6709-6716.	5.2	54
95	Adsorption and migration of carbon adatoms on zigzag carbon nanotubes. Carbon, 2004, 42, 1021-1025.	5.4	52
96	Creating nanoporous graphene with swift heavy ions. Carbon, 2017, 114, 511-518.	5.4	52
97	Strains Induced by Point Defects in Graphene on a Metal. Physical Review Letters, 2013, 111, 085501.	2.9	51
98	Phosphorene under electron beam: from monolayer to one-dimensional chains. Nanoscale, 2016, 8, 7949-7957.	2.8	51
99	Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering. Science Advances, 2021, 7, .	4.7	51
100	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
101	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
102	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></mm from molecular dynamics using different empirical potentials. Physical Review B, 2019, 99, .	1.1	50
103	Irradiation-induced stiffening of carbon nanotube bundles. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 142-145.	0.6	49
104	Gold-embedded zigzag graphene nanoribbons as spin gapless semiconductors. Physical Review B, 2012, 86, .	1.1	48
105	Multiwalled carbon nanotubes as apertures and conduits for energetic ions. Physical Review B, 2005, 71, .	1.1	47
106	Relative abundance of single and double vacancies in irradiated single-walled carbon nanotubes. Applied Physics Letters, 2007, 91, 173109.	1.5	45
107	Structural Distortions and Charge Density Waves in Iodine Chains Encapsulated inside Carbon Nanotubes. Nano Letters, 2017, 17, 3694-3700.	4.5	44
108	The diffusion of carbon atoms inside carbon nanotubes. New Journal of Physics, 2008, 10, 023022.	1.2	42

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109	Modifying the electronic structure of semiconducting single-walled carbon nanotubes byAr+ion irradiation. Physical Review B, 2009, 79, .	1.1	42
110	Ion irradiation tolerance of graphene as studied by atomistic simulations. Applied Physics Letters, 2012, 100, 233108.	1.5	42
111	Perforating Freestanding Molybdenum Disulfide Monolayers with Highly Charged Ions. Journal of Physical Chemistry Letters, 2019, 10, 904-910.	2.1	42
112	Migration of gold atoms in graphene ribbons: Role of the edges. Physical Review B, 2010, 81, .	1.1	41
113	Chiralityâ€Dependent Reactivity of Individual Singleâ€Walled Carbon Nanotubes. Small, 2013, 9, 1379-1386.	5.2	41
114	Layer-Dependent Band Gaps of Platinum Dichalcogenides. ACS Nano, 2021, 15, 13249-13259.	7.3	41
115	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
116	Electron-Beam-Driven Structure Evolution of Single-Layer MoTe₂ for Quantum Devices. ACS Applied Nano Materials, 2019, 2, 3262-3270.	2.4	39
117	Carbon nanotubes as masks against ion irradiation: An insight from atomistic simulations. Applied Physics Letters, 2002, 81, 1101-1103.	1.5	37
118	Fabrication and atomic structure of size-selected, layered MoS₂clusters for catalysis. Nanoscale, 2014, 6, 12463-12469.	2.8	37
119	Predicted scanning tunneling microscopy images of carbon nanotubes with atomic vacancies. Solid State Communications, 2001, 118, 361-365.	0.9	36
120	Enhanced sensitivity of MoSe₂ monolayer for gas adsorption induced by electric field. Journal of Physics Condensed Matter, 2019, 31, 445301.	0.7	35
121	Data-Driven Quest for Two-Dimensional Non-van der Waals Materials. Nano Letters, 2022, 22, 989-997.	4.5	35
122	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
123	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
124	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. Physical Review B, 2011, 84, .	1.1	32
125	Xe irradiation of graphene on Ir(111): From trapping to blistering. Physical Review B, 2015, 92, .	1.1	32
126	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></r Mirror-Twin Boundaries. Physical Review X, 2019, 9, .	2.8	32

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127	<i>In Situ</i> Growth of Cellular Two-Dimensional Silicon Oxide on Metal Substrates. ACS Nano, 2013, 7, 5175-5180.	7.3	31
128	A first-principles study on magnetic coupling between carbon adatoms on graphene. New Journal of Physics, 2010, 12, 113021.	1.2	30
129	Alkali metals inside bi-layer graphene and MoS2: Insights from first-principles calculations. Nano Energy, 2020, 75, 104927.	8.2	30
130	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
131	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
132	Channeling of heavy ions through multi-walled carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 21-25.	0.6	29
133	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
134	Growth of Singleâ€Walled Carbon Nanotubes from Sharp Metal Tips. Small, 2009, 5, 2710-2715.	5.2	29
135	Interfacial Carbon Nanoplatelet Formation by Ion Irradiation of Graphene on Iridium(111). ACS Nano, 2014, 8, 12208-12218.	7.3	29
136	Stopping of energetic ions in carbon nanotubes. Nuclear Instruments & Methods in Physics Research B, 2003, 206, 18-21.	0.6	28
137	Coronene Encapsulation in Singleâ€Walled Carbon Nanotubes: Stacked Columns, Peapods, and Nanoribbons. ChemPhysChem, 2014, 15, 1660-1665.	1.0	28
138	Making junctions between carbon nanotubes using an ion beam. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 224-229.	0.6	27
139	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
140	Simulating Raman spectra by combining first-principles and empirical potential approaches with application to defective MoS2. Npj Computational Materials, 2020, 6, .	3.5	27
141	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
142	Swift chemical sputtering of covalently bonded materials. Pure and Applied Chemistry, 2006, 78, 1203-1211.	0.9	26
143	Response of mechanically strained nanomaterials to irradiation: Insight from atomistic simulations. Physical Review B, 2010, 82, .	1.1	26
144	Are two-dimensional materials radiation tolerant?. Nanoscale Horizons, 2020, 5, 1447-1452.	4.1	26

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145	Band Bending and Valence Band Quantization at Line Defects in MoS₂. ACS Nano, 2020, 14, 9176-9187.	7.3	26
146	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
147	Local vibrational modes of Si vacancy spin qubits in SiC. Physical Review B, 2020, 101, .	1.1	25
148	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
149	Observation of charge density waves in free-standing 1T-TaSe2 monolayers by transmission electron microscopy. Applied Physics Letters, 2018, 113, .	1.5	24
150	Silicon and silicon-nitrogen impurities in graphene: Structure, energetics, and effects on electronic transport. Physical Review B, 2015, 92, .	1.1	23
151	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
152	Electrical properties of C⁴⁺ irradiated singleâ€walled carbon nanotube paper. Physica Status Solidi (B): Basic Research, 2008, 245, 2280-2283.	0.7	21
153	When defects are not defects. Nature Materials, 2018, 17, 757-758.	13.3	21
154	Enhanced Trion Emission in Monolayer MoSe₂ by Constructing a Typeâ€I Van Der Waals Heterostructure. Advanced Functional Materials, 2021, 31, 2104960.	7.8	21
155	Chlorine doping of MoSe₂ flakes by ion implantation. Nanoscale, 2021, 13, 5834-5846.	2.8	21
156	Edge and Pointâ€Defect Induced Electronic and Magnetic Properties in Monolayer PtSe₂. Advanced Functional Materials, 2022, 32, .	7.8	21
157	Structure and stability of non-molecular nitrogen at ambient pressure. Europhysics Letters, 2004, 65, 400-406.	0.7	20
158	From Permeation to Cluster Arrays: Graphene on Ir(111) Exposed to Carbon Vapor. Nano Letters, 2017, 17, 3105-3112.	4.5	20
159	Defect-induced junctions between single- or double-wall carbon nanotubes and metal crystals. Nanoscale, 2010, 2, 901.	2.8	19
160	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
161	Mechanical properties and current-carrying capacity of Al reinforced with graphene/BN nanoribbons: a computational study. Nanoscale, 2016, 8, 20080-20089.	2.8	19
162	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

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163	Molecular dynamics simulations of CH3 sticking on carbon surfaces. Journal of Applied Physics, 2003, 93, 1826-1831.	1.1	18
164	Vibrational Properties of a Two-Dimensional Silica Kagome Lattice. ACS Nano, 2016, 10, 10929-10935.	7.3	18
165	Nitrogen-doped carbon nanotubes under electron irradiation simulated with a tight-binding model. Physical Review B, 2006, 74, .	1.1	17
166	Atomistic simulations of irradiation effects in carbon nanotubes: an overview. Radiation Effects and Defects in Solids, 2007, 162, 157-169.	0.4	17
167	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: An<i>ab initio</i>study. Physical Review B, 2010, 82, .	1.1	17
168	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
169	Study of acoustic emission signals during fracture shear deformation. Acoustical Physics, 2016, 62, 505-513.	0.2	17
170	Hydrogen-assisted post-growth substitution of tellurium into molybdenum disulfide monolayers with tunable compositions. Nanotechnology, 2018, 29, 145603.	1.3	17
171	Reversible crystalline-to-amorphous phase transformation in monolayer MoS2 under grazing ion irradiation. 2D Materials, 2020, 7, 025005.	2.0	17
172	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
173	Computational study of boron nitride nanotube synthesis: How catalyst morphology stabilizes the boron nitride bond. Physical Review B, 2009, 80, .	1.1	16
174	Luminescence of defects in the structural transformation of layered tin dichalcogenides. Applied Physics Letters, 2017, 111, .	1.5	16
175	Freestanding and Supported MoS₂ Monolayers under Cluster Irradiation: Insights from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2020, 12, 37454-37463.	4.0	16
176	Photoluminescence line shapes for color centers in silicon carbide from density functional theory calculations. Physical Review B, 2021, 103, .	1.1	16
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