Abhishek K Singh

List of Publications by Year
in descending order

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172	8,946	43973 48	48187 88
papers	citations	h-index	g-index

175	175	175	11562
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Feature Blending: An Approach toward Generalized Machine Learning Models for Property Prediction. ACS Physical Chemistry Au, 2022, 2, 16-22.	1.9	6
2	Diffusion-enhanced preferential growth of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e570" altimg="si37.svg"><mml:mi>m</mml:mi></mml:math>-oriented GaN micro-domains on directly grown graphene with a large domain size on Ti/SiO2/Si(001). Materials Today Communications, 2022, 30, 103113.	0.9	3
3	Layer parity dependent Raman-active modes and crystal symmetry in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">ReS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2022, 105, .	1.1	5
4	Tuning Catalytic Activity in Ultrathin Bimetallic Nanowires via Surface Segregation: Some Insights. Journal of Physical Chemistry Letters, 2022, 13, 770-776.	2.1	0
5	Interfacial Electron Transfer Strategy to Improve the Hydrogen Evolution Catalysis of CrP Heterostructure. Small, 2022, 18, e2106139.	5.2	9
6	Electroreduction of CO₂ with Tunable Selectivity on Auâ€“Pd Bimetallic Catalyst: A First Principle Study. ACS Applied Materials & Interfaces, 2022, 14, 11313-11321.	4.0	4
7	Noble-Metal-Free Heterojunction Photocatalyst for Selective CO₂ Reduction to Methane upon Induced Strain Relaxation. ACS Catalysis, 2022, 12, 687-697.	5.5	56
8	Origin of layer-dependent electrical conductivity of transition metal dichalcogenides. Physical Review B, 2022, 105, .	1.1	5
9	Quantum confinement effect on defect level of hydrogen doped rutile VO2 nanowires. Journal of Applied Physics, 2022, 131, .	1.1	4
10	Growth of highly crystalline ultrathin two-dimensional selenene. 2D Materials, 2022, 9, 045004.	2.0	8
11	Decoupled atomic contribution boosted high thermoelectric performance in mixed cation spinel oxides ACo2O4. Applied Physics Letters, 2022, 120, .	1.5	4
12	Improvement in Oxygen Evolution Performance of NiFe Layered Double Hydroxide Grown in the Presence of 1T-Rich MoS₂. ACS Applied Materials & Interfaces, 2022, 14, 31951-31961.	4.0	8
13	Nonlinear Optical Absorption of ReS₂ Driven by Stacking Order. ACS Photonics, 2021, 8, 405-411.	3.2	16
14	Accelerated Discovery of Thermoelectric Materials Using Machine Learning. Springer Series in Materials Science, 2021, , 133-152.	0.4	1
15	Mechanistic study on nitrogen-doped graphitic carbon-reinforced chromium nitride as a durable electrocatalyst for oxygen reduction. Journal of Materials Chemistry A, 2021, 9, 16575-16584.	5.2	14
16	Anisotropic Interlayer Exciton in GeSe/SnS van der Waals Heterostructure. Journal of Physical Chemistry Letters, 2021, 12, 1765-1771.	2.1	11
17	Ultralow Thermal Conductivity in Earth-Abundant Cu_{1.6}Bi_{4.8}S₈: Anharmonic Rattling of Interstitial Cu. Chemistry of Materials, 2021, 33, 2993-3001.	3.2	26
18	Emerging 2D metal oxides and their applications. Materials Today, 2021, 45, 142-168.	8.3	164

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19	Formation of a Small Electron Polaron in Tantalum Oxynitride: Origin of Low Mobility. Journal of Physical Chemistry C, 2021, 125, 11548-11554.	1.5	16
20	Rational Design of Single-Atom Catalysts for Enhanced Electrocatalytic Nitrogen Reduction Reaction. Journal of Physical Chemistry C, 2021, 125, 12585-12593.	1.5	20
21	Atypical behavior of intrinsic defects and promising dopants in two-dimensional <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>WS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review Materials, 2021, 5, .	3.1	10
22	Accelerated Discovery of the Valley-Polarized Quantum Anomalous Hall Effect in MXenes. Chemistry of Materials, 2021, 33, 6311-6317.	3.2	18
23	Electrooxidation of Hydrazine Utilizing High-Entropy Alloys: Assisting the Oxygen Evolution Reaction at the Thermodynamic Voltage. ACS Catalysis, 2021, 11, 14000-14007.	5.5	47
24	Chemical hardness-driven interpretable machine learning approach for rapid search of photocatalysts. Npj Computational Materials, 2021, 7, .	3.5	40
25	Electroreduction of Carbon Dioxide into Selective Hydrocarbons at Low Overpotential Using Isomorphic Atomic Substitution in Copper Oxide. ACS Sustainable Chemistry and Engineering, 2020, 8, 179-189.	3.2	11
26	Pressureâ€Dependent Behavior of Defectâ€Modulated Band Structure in Boron Arsenide. Advanced Materials, 2020, 32, e2001942.	11.1	18
27	Inner Sphere Electron Transfer Promotion on Homogeneously Dispersed Fe-N_x Centers for Energy-Efficient Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 36026-36039.	4.0	39
28	Electronic Structure Based Intuitive Design Principle of Singleâ€Atom Catalysts for Efficient Electrolytic Nitrogen Reduction. ChemCatChem, 2020, 12, 5456-5464.	1.8	16
29	Development of Vickers hardness prediction models via microstructural analysis and machine learning. Journal of Materials Science, 2020, 55, 15845-15856.	1.7	30
30	Multi-component (Agâ€“Auâ€“Cuâ€“Pdâ€“Pt) alloy nanoparticle-decorated p-type 2D-molybdenum disulfide (MoS₂) for enhanced hydrogen sensing. Nanoscale, 2020, 12, 11830-11841.	2.8	42
31	Nanostructured Tungsten Oxysulfide as an Efficient Electrocatalyst for Hydrogen Evolution Reaction. ACS Catalysis, 2020, 10, 6753-6762.	5.5	43
32	Formic acid and methanol electro-oxidation and counter hydrogen production using nano high entropy catalyst. Materials Today Energy, 2020, 16, 100393.	2.5	38
33	Unraveling the role of bonding chemistry in connecting electronic and thermal transport by machine learning. Journal of Materials Chemistry A, 2020, 8, 8716-8721.	5.2	21
34	Ultralow thermal conductivity and high thermoelectric figure of merit in mixed valence In₅X₅Br (X = S, and Se) compounds. Journal of Materials Chemistry A, 2020, 8, 13812-13819.	5.2	16
35	A Statistical Approach for the Rapid Prediction of Electron Relaxation Time Using Elemental Representatives. Chemistry of Materials, 2020, 32, 6507-6514.	3.2	22
36	Accelerated prediction of Vickers hardness of Co- and Ni-based superalloys from microstructure and composition using advanced image processing techniques and machine learning. Acta Materialia, 2020, 196, 295-303.	3.8	40

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37	Carrier Dynamics in Ultrathin Gold Nanowires: Role of Auger Processes. Plasmonics, 2020, 15, 1151-1158.	1.8	2
38	Guided patchwork kriging to develop highly transferable thermal conductivity prediction models. JPhys Materials, 2020, 3, 024006.	1.8	13
39	High-Entropy Alloys as Catalysts for the CO₂ and CO Reduction Reactions: Experimental Realization. ACS Catalysis, 2020, 10, 3658-3663.	5.5	244
40	Strong Chemical Bond Hierarchy Leading to Exceptionally High Thermoelectric Figure of Merit in Oxychalcogenide AgBiTeO. ACS Applied Materials & Interfaces, 2020, 12, 8280-8287.	4.0	26
41	Stackingâ€Orderâ€Driven Optical Properties and Carrier Dynamics in ReS₂. Advanced Materials, 2020, 32, e1908311.	11.1	38
42	Coupling the High-Throughput Property Map to Machine Learning for Predicting Lattice Thermal Conductivity. Chemistry of Materials, 2019, 31, 5145-5151.	3.2	63
43	Rattling-Induced Ultralow Thermal Conductivity Leading to Exceptional Thermoelectric Performance in AgIn₅S₈. ACS Applied Materials & Interfaces, 2019, 11, 33894-33900.	4.0	25
44	Critical Sublattice Symmetry Breaking: A Universal Criterion for Dirac Cone Splitting. Journal of Physical Chemistry C, 2019, 123, 23082-23088.	1.5	2
45	Topological Phases in Hydrogenated Group 13 Monolayers. Journal of Physical Chemistry C, 2019, 123, 25985-25990.	1.5	4
46	Recent advances in MXenes: From fundamentals to applications. Current Opinion in Solid State and Materials Science, 2019, 23, 164-178.	5.6	247
47	Morphology controlled synthesis of low bandgap SnSe₂ with high photodetectivity. Nanoscale, 2019, 11, 870-877.	2.8	31
48	Structureâ€Dependent Electrical and Magnetic Properties of Iron Oxide Composites. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1801004.	0.8	3
49	Thermal Conductivity Enhancement in <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></mml:mrow></mml:msub></mml:mrow></mml:math> under Extreme Strain. Physical Review Letters, 2019, 122, 155901.	2.9	75
50	Origin of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math> -type conductivity of 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> Physical Review B, 2019, 99, .	1.1	72
51	Magnetism in two-dimensional materials beyond graphene. Materials Today, 2019, 27, 107-122.	8.3	127
52	Accelerated Data-Driven Accurate Positioning of the Band Edges of MXenes. Journal of Physical Chemistry Letters, 2019, 10, 780-785.	2.1	43
53	Origin of Ultralow Thermal Conductivity in n-Type Cubic Bulk AgBiS₂: Soft Ag Vibrations and Local Structural Distortion Induced by the Bi 6s² Lone Pair. Chemistry of Materials, 2019, 31, 2106-2113.	3.2	70
54	Revealing carbon mediated luminescence centers with enhanced lifetime in porous alumina. Journal of Applied Physics, 2019, 126, 164904.	1.1	6

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55	Noninvasive Subsurface Electrical Probe for Encapsulated Layers in van der Waals Heterostructures. Physical Review Applied, 2019, 12, .	1.5	7
56	An amine functionalized zirconium metalâ€“organic framework as an effective chemiresistive sensor for acidic gases. Chemical Communications, 2019, 55, 349-352.	2.2	83
57	Atomically thin gallium layers from solid-melt exfoliation. Science Advances, 2018, 4, e1701373.	4.7	157
58	Pressure-Induced Topological Phase Transitions in CdGeSb₂ and CdSnSb₂. Journal of Physical Chemistry Letters, 2018, 9, 2202-2207.	2.1	14
59	C2N/WS2 van der Waals type-II heterostructure as a promising water splitting photocatalyst. Journal of Catalysis, 2018, 359, 143-150.	3.1	229
60	Origamiâ€Inspired 3D Interconnected Molybdenum Carbide Nanoflakes. Advanced Materials Interfaces, 2018, 5, 1701113.	1.9	13
61	Interplay of Structural and Bonding Characters in Thermal Conductivity and Born-Effective Charge of Transition Metal Dichalcogenides. Journal of Physical Chemistry C, 2018, 122, 2521-2527.	1.5	7
62	Structural, vibrational, and electronic topological transitions of Bi1.5Sb0.5Te1.8Se1.2 under pressure. Journal of Applied Physics, 2018, 123, .	1.1	14
63	Towards band structure and band offset engineering of monolayer Mo _(1â^' x) W _(x) S ₂ via Strain. 2D Materials, 2018, 5, 015008.	2.0	28
64	Effective sensing radius (ESR) and performance analysis of static and mobile sensor networks. Telecommunication Systems, 2018, 68, 115-127.	1.6	9
65	Graphene Oxide Epoxy (GOâ€xy): GO as Epoxy Adhesive by Interfacial Reaction of Functionalities. Advanced Materials Interfaces, 2018, 5, 1700657.	1.9	19
66	Synergistic coreâ€“shell interactions enable ultra-low overpotentials for enhanced CO₂ electro-reduction activity. Journal of Materials Chemistry A, 2018, 6, 21120-21130.	5.2	10
67	High Thermoelectric Figure of Merit via Tunable Valley Convergence Coupled Low Thermal Conductivity in AIIBIVC2VChalcopyrites. Journal of Physical Chemistry C, 2018, 122, 29150-29157.	1.5	25
68	An Insight into the Phase Transformation of WS₂ upon Fluorination. Advanced Materials, 2018, 30, e1803366.	11.1	26
69	Engineering Defect Transition-Levels through the van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 24475-24480.	1.5	27
70	Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene. Chemistry of Materials, 2018, 30, 4031-4038.	3.2	235
71	Nonlinear Polarization and Low-Dissipation Ultrafast Optical Switching in Phosphorene. Journal of Physical Chemistry C, 2018, 122, 19146-19152.	1.5	5
72	Reflection and Transmission of P-Waves in an Intermediate Layer Lying Between Two Semi-infinite Media. Pure and Applied Geophysics, 2018, 175, 4305-4319.	0.8	6

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73	A Non-van der Waals Two-Dimensional Material from Natural Titanium Mineral Ore Ilmenite. Chemistry of Materials, 2018, 30, 5923-5931.	3.2	82
74	Multiple triple-point fermions in Heusler compounds. Journal of Physics Condensed Matter, 2018, 30, 375702.	0.7	8
75	Manipulation of Optoelectronic Properties and Band Structure Engineering of Ultrathin Te Nanowires by Chemical Adsorption. ACS Applied Materials & Interfaces, 2017, 9, 19462-19469.	4.0	9
76	Growth of Molybdenum Carbideâ€“Graphene Hybrids from Molybdenum Disulfide Atomic Layer Template. Advanced Materials Interfaces, 2017, 4, 1600866.	1.9	14
77	Strain-induced indirect-to-direct band-gap transition in bulk <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SnS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2017, 95, .	1.1	49
78	Structural and spectroscopic characterizations of a new near-UV-converting cyan-emitting RbBaScSi3O9:Eu2+ phosphor with robust thermal performance. Journal of Alloys and Compounds, 2017, 713, 138-147.	2.8	24
79	High Thermoelectric Performance in n-Doped Silicon-Based Chalcogenide Si₂Te₃. Chemistry of Materials, 2017, 29, 3723-3730.	3.2	34
80	Hydrogen Evolution Reaction Activity of Grapheneâ€“MoS₂ van der Waals Heterostructures. ACS Energy Letters, 2017, 2, 1355-1361.	8.8	141
81	Orientation Selection during Heterogeneous Nucleation: Implications for Heterogeneous Catalysis. Journal of Physical Chemistry C, 2017, 121, 10027-10037.	1.5	13
82	Effect of Cr addition on Î³â€“Î³â€² cobalt-based Coâ€“Moâ€“Alâ€“Ta class of superalloys: a combined experimental and computational study. Journal of Materials Science, 2017, 52, 11036-11047.	1.7	61
83	Negative differential resistance in armchair silicene nanoribbons. Nanotechnology, 2017, 28, 275402.	1.3	6
84	Topologically nontrivial electronic states in CaSn3. Journal of Applied Physics, 2017, 121, .	1.1	14
85	Ferroelectricity, Antiferroelectricity, and Ultrathin 2D Electron/Hole Gas in Multifunctional Monolayer MXene. Nano Letters, 2017, 17, 3290-3296.	4.5	184
86	Fluorinated h-BN as a magnetic semiconductor. Science Advances, 2017, 3, e1700842.	4.7	121
87	Atomistic Origin of Phase Stability in Oxygen-Functionalized MXene: A Comparative Study. Journal of Physical Chemistry C, 2017, 121, 18947-18953.	1.5	44
88	Monolayer BC₂: an ultrahigh capacity anode material for Li ion batteries. Physical Chemistry Chemical Physics, 2017, 19, 24230-24239.	1.3	29
89	Existence of Ti²⁺ States on the Surface of Heavily Reduced SrTiO₃ Nanocubes. Chemistry of Materials, 2017, 29, 9887-9891.	3.2	14
90	Insights into nucleation, growth and phase selection of WO₃: morphology control and electrochromic properties. Journal of Materials Chemistry C, 2017, 5, 7307-7316.	2.7	34

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91	Metalâ€Free Dual Modal Contrast Agents Based on Fluorographene Quantum Dots. Particle and Particle Systems Characterization, 2017, 34, 1600221.	1.2	25
92	Simultaneous Site Adsorption Shift and Efficient CO Oxidation Induced by V and Co in Pt Catalyst. Journal of Physical Chemistry C, 2017, 121, 12807-12816.	1.5	15
93	Pressureâ€Induced Charge Transfer Doping of Monolayer Graphene/MoS₂ Heterostructure. Small, 2016, 12, 4063-4069.	5.2	45
94	Effect of ambient on electrical transport properties of ultra-thin Au nanowires. Applied Physics Letters, 2016, 109, 253108.	1.5	4
95	â€œCappingâ€•out oxygen interference: An approach to achieve efficient hydrogen storage via Kubas binding. International Journal of Hydrogen Energy, 2016, 41, 5979-5985.	3.8	5
96	Diffusive nature of thermal transport in stanene. Physical Chemistry Chemical Physics, 2016, 18, 14257-14263.	1.3	34
97	Interferroelectric transition as another manifestation of intrinsic size effect in ferroelectrics. Physical Review B, 2016, 94, .	1.1	8
98	Strain-induced chiral symmetry breaking leads to large Dirac cone splitting in graphene/graphane heterostructure. Physical Review B, 2016, 94, .	1.1	18
99	Mechanistic Insight into the Chemical Exfoliation and Functionalization of Ti₃C₂ MXene. ACS Applied Materials & Interfaces, 2016, 8, 24256-24264.	4.0	221
100	Suppression of Jahnâ€“Teller Distortions and Origin of Piezochromism and Thermochromism in Cuâ€“Cl Hybrid Perovskite. Inorganic Chemistry, 2016, 55, 6817-6824.	1.9	24
101	Isolation of pristine MXene from Nb₄AlC₃ MAX phase: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 11073-11080.	1.3	47
102	Simultaneous tunability of the electronic and phononic gaps in SnS ₂ under normal compressive strain. 2D Materials, 2016, 3, 015009.	2.0	16
103	Simultaneous enhancement of electrical conductivity and thermopower in Bi₂S₃ under hydrostatic pressure. Journal of Materials Chemistry C, 2016, 4, 1979-1987.	2.7	19
104	Lifshitz transition and modulation of electronic and transport properties of bilayer graphene by sliding and applied normal compressive strain. Carbon, 2016, 99, 432-438.	5.4	22
105	Ultra-sensitive pressure dependence of bandgap of rutile-GeO2 revealed by many body perturbation theory. Journal of Chemical Physics, 2015, 143, 064703.	1.2	9
106	High temperature thermoelectric properties of Zr and Hf based transition metal dichalcogenides: A first principles study. Journal of Chemical Physics, 2015, 143, 234704.	1.2	72
107	High thermopower and ultra low thermal conductivity in Cd-based Zintl phase compounds. Physical Chemistry Chemical Physics, 2015, 17, 16917-16926.	1.3	33
108	Strain-induced phenomena in layered materials. , 2015, , .		0

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109	Pt-Poisoning-Free Efficient CO Oxidation on Pt₃Co Supported on MgO(100): An Ab Initio Study. ACS Catalysis, 2015, 5, 1826-1832.	5.5	20
110	Semiconductor to metal transition in bilayer phosphorene under normal compressive strain. Nanotechnology, 2015, 26, 075701.	1.3	83
111	A new class of high strength high temperature Cobalt based Î³â€“Î³â€² Coâ€“Moâ€“Al alloys stabilized with Ta addition. Acta Materialia, 2015, 97, 29-40.	3.8	151
112	Vacancy mediated clipping of multi-layered graphene: A precursor for 1, 2 and 3D carbon structures. Carbon, 2015, 94, 67-72.	5.4	5
113	Graphene-oxide-supported ultrathin Au nanowires: efficient electrocatalysts for borohydride oxidation. Chemical Communications, 2015, 51, 16856-16859.	2.2	17
114	Remarkable enhancement in hydrogen storage on free-standing Ti 3 B and BC 3 supported Ti 3 clusters. International Journal of Hydrogen Energy, 2015, 40, 1054-1061.	3.8	22
115	Pressure-Dependent Optical and Vibrational Properties of Monolayer Molybdenum Disulfide. Nano Letters, 2015, 15, 346-353.	4.5	284
116	First Principles Study on Structural Stability of Belite. ACI Materials Journal, 2015, 112, .	0.3	3
117	Enhancing hydrogen storage capacity of pyridine-based metal organic framework. International Journal of Hydrogen Energy, 2014, 39, 9293-9299.	3.8	6
118	Pressure-induced semiconducting to metallic transition in multilayered molybdenum disulphide. Nature Communications, 2014, 5, 3731.	5.8	495
119	Effect of strain on electronic and thermoelectric properties of few layers to bulk MoS₂. Nanotechnology, 2014, 25, 465701.	1.3	101
120	Strain-induced electronic phase transition and strong enhancement of thermopower of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">TiS</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	24
121	Pressure induced manifold enhancement of Li-kinetics in FCC fullerene. Physical Chemistry Chemical Physics, 2014, 16, 21688-21693.	1.3	3
122	Mechanical and electronic properties of pristine and Ni-doped Si, Ge, and Sn sheets. Physical Chemistry Chemical Physics, 2014, 16, 1667-1671.	1.3	46
123	Origin of enhanced thermoelectric properties of doped CrSi₂. RSC Advances, 2014, 4, 3482-3486.	1.7	8
124	Semiconductor-like Sensitivity in Metallic Ultrathin Gold Nanowire-Based Sensors. Journal of Physical Chemistry C, 2014, 118, 18676-18682.	1.5	17
125	Boron doped defective graphene as a potential anode material for Li-ion batteries. Physical Chemistry Chemical Physics, 2014, 16, 16502.	1.3	111
126	Wrinkling of Atomic Planes in Ultrathin Au Nanowires. Nano Letters, 2014, 14, 4859-4866.	4.5	35

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127	Low formation energy and kinetic barrier of Stoneâ€“Wales defect in infinite and finite silicene. Chemical Physics Letters, 2014, 592, 52-55.	1.2	22
128	pentahexoctite: A new two-dimensional allotrope of carbon. Scientific Reports, 2014, 4, 7164.	1.6	85
129	Li diffusion through doped and defected graphene. Physical Chemistry Chemical Physics, 2013, 15, 15128.	1.3	86
130	New insights into designing metallacarborane based room temperature hydrogen storage media. Journal of Chemical Physics, 2013, 139, 164319.	1.2	20
131	Electronic transport in patterned graphene nanoroads. Nanotechnology, 2013, 24, 495201.	1.3	10
132	Thermoelectric properties of Î²-FeSi2. Journal of Applied Physics, 2013, 114, .	1.1	23
133	Mechanism for the Compressive Strain Induced Oscillations in the Conductance of Carbon Nanotubes. Physical Review Letters, 2013, 110, 095504.	2.9	7
134	Single crystalline ultrathin gold nanowires: Promising nanoscale interconnects. AIP Advances, 2013, 3, .	0.6	25
135	Effect of the Edge Type and Strain on the Structural, Electronic and Magnetic Properties of the BNRs. Journal of Nanoscience and Nanotechnology, 2012, 12, 1899-1902.	0.9	1
136	Semiconductor-metal transition in semiconducting bilayer sheets of transition-metal dichalcogenides. Physical Review B, 2012, 86, .	1.1	259
137	First principles calculations of H-storage in sorption materials. Journal of Materials Science, 2012, 47, 7356-7366.	1.7	33
138	Hydrogen Storage Capacity of Carbon-Foams: Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2011, 115, 2476-2482.	1.5	51
139	Insulating State and Breakdown of Fermi Liquid Description in Molecular-Scale Single-Crystalline Wires of Gold. ACS Nano, 2011, 5, 8398-8403.	7.3	36
140	Quantum Dots and Nanoroads of Graphene Embedded in Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2011, 115, 9889-9893.	1.5	135
141	Calcium-Decorated Carbyne Networks as Hydrogen Storage Media. Nano Letters, 2011, 11, 2660-2665.	4.5	98
142	Armchair or Zigzag? A tool for characterizing graphene edge. Computer Physics Communications, 2011, 182, 804-807.	3.0	9
143	Patterning nanoroads and quantum dots on fluorinated graphene. Nano Research, 2011, 4, 143-152.	5.8	120
144	Metallacarboranes: Toward Promising Hydrogen Storage Metal Organic Frameworks. Journal of the American Chemical Society, 2010, 132, 14126-14129.	6.6	55

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145	Vacancy Clusters in Graphane as Quantum Dots. ACS Nano, 2010, 4, 3510-3514.	7.3	119
146	The influence of insulating substrate on the electrical measurements of focused ion beam fabricated electrodes with nano-gap spacing. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3282-3286.	0.6	4
147	The ultimate diamond slab: GraphAne versus graphEne. Diamond and Related Materials, 2010, 19, 368-373.	1.8	71
148	Electronics and Magnetism of Patterned Graphene Nanoroads. Nano Letters, 2009, 9, 1540-1543.	4.5	235
149	Hydrogen interactions with acceptor impurities in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SnO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: First-principles calculations. Physical Review B, 2009, 79, .	1.1	63
150	H-Spillover through the Catalyst Saturation: An Ab Initio Thermodynamics Study. ACS Nano, 2009, 3, 1657-1662.	7.3	127
151	Sources of Electrical Conductivity in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SnO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2008, 101, 055502.	2.9	352
152	THEORETICAL ADVANCES IN THE ELECTRONIC AND ATOMIC STRUCTURES OF SILICON NANOTUBES AND NANOWIRES. , 2008, , 217-257.		2
153	Probing Properties of Boron Î±-Tubes by Ab Initio Calculations. Nano Letters, 2008, 8, 1314-1317.	4.5	140
154	The Boron Buckyball and Its Precursors: An Electronic Structure Study. Journal of Physical Chemistry A, 2008, 112, 13679-13683.	1.1	57
155	Clustering of Sc on SWNT and Reduction of Hydrogen Uptake:â€‰ Ab-Initio All-Electron Calculations. Journal of Physical Chemistry C, 2007, 111, 17977-17980.	1.5	159
156	Charged and magnetic fullerenes of silicon by metal encapsulation: Predictions fromab initiocalculations. Physical Review B, 2006, 74, .	1.1	47
157	Effects of Morphology and Doping on the Electronic and Structural Properties of Hydrogenated Silicon Nanowires. Nano Letters, 2006, 6, 920-925.	4.5	78
158	Structural and magnetic stabilities of cubic and orthorhombic phases of CeMnNi4. Applied Physics Letters, 2006, 89, 222502.	1.5	11
159	Metal encapsulated nanotubes of germanium with metal dependent electronic properties. European Physical Journal D, 2005, 34, 295-298.	0.6	11
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