

Rajeev Ahuja

List of Publications by Year in descending order

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976
papers

37,827
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4146

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30322
citing authors

#	ARTICLE	IF	CITATIONS
1	Ferromagnetism above room temperature in bulk and transparent thin films of Mn-doped ZnO. <i>Nature Materials</i> , 2003, 2, 673-677.	27.5	1,687
2	Defect Engineered g-C ₃ N ₄ for Efficient Visible Light Photocatalytic Hydrogen Production. <i>Chemistry of Materials</i> , 2015, 27, 4930-4933.	6.7	401
3	Calculated elastic properties of M ₂ AlC (M=Ti, V, Cr, Nb and Ta). <i>Solid State Communications</i> , 2004, 129, 589-592.	1.9	397
4	Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26560-26568.	3.1	383
5	Experimental evidence for sub-3-fs charge transfer from an aromatic adsorbate to a semiconductor. <i>Nature</i> , 2002, 418, 620-623.	27.8	346
6	Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. <i>Catalysis Science and Technology</i> , 2017, 7, 545-559.	4.1	345
7	Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS ₂ /AlN(GaN) Heterostructures. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17594-17599.	3.1	340
8	Electronic, bonding, and optical properties of CeO ₂ and Ce ₂ O ₃ from first principles. <i>Physical Review B</i> , 2001, 64, .	3.2	337
9	The hardest known oxide. <i>Nature</i> , 2001, 410, 653-654.	27.8	316
10	Phonon related properties of transition metals, their carbides, and nitrides: A first-principles study. <i>Journal of Applied Physics</i> , 2007, 101, 123519.	2.5	312
11	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. <i>ChemSusChem</i> , 2015, 8, 2789-2825.	6.8	302
12	Physisorption of nucleobases on graphene: Density-functional calculations. <i>Physical Review B</i> , 2007, 76, .	3.2	296
13	Cubic Hf ₃ N ₄ and Zr ₃ N ₄ : A class of hard materials. <i>Physical Review B</i> , 2003, 68, .	3.2	294
14	Structure of Phase Change Materials for Data Storage. <i>Physical Review Letters</i> , 2006, 96, 055507.	7.8	293
15	Single-layer MoS ₂ as an efficient photocatalyst. <i>Catalysis Science and Technology</i> , 2013, 3, 2214.	4.1	271
16	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. <i>Materials Today</i> , 2020, 32, 108-130.	14.2	271
17	The Importance of Strong Carbon~Metal Adhesion for Catalytic Nucleation of Single-Walled Carbon Nanotubes. <i>Nano Letters</i> , 2008, 8, 463-468.	9.1	269
18	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. <i>Physical Review B</i> , 1996, 53, 3072-3079.	3.2	259

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19	Quasi-Ab Initio Molecular Dynamic Study of Fe Melting. Physical Review Letters, 2000, 84, 3638-3641.	7.8	248
20	Li-decorated metal-organic framework 5: A route to achieving a suitable hydrogen storage medium. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20173-20176.	7.1	232
21	Bonding and classification of nanolayered ternary carbides. Physical Review B, 2004, 70, .	3.2	212
22	Mn+1AX _n phases in the Ti-Si-C system studied by thin-film synthesis and ab initio calculations. Physical Review B, 2004, 70, .	3.2	212
23	Deposition and characterization of ternary thin films within the Ti-Al-C system by DC magnetron sputtering. Journal of Crystal Growth, 2006, 291, 290-300.	1.5	212
24	Stability of the body-centred-cubic phase of iron in the Earth's inner core. Nature, 2003, 424, 1032-1034.	27.8	201
25	Carbon Nanomaterials as Catalysts for Hydrogen Uptake and Release in NaAlH ₄ . Nano Letters, 2009, 9, 1501-1505.	9.1	200
26	Magnetism and band gap narrowing in Cu-doped ZnO. Applied Physics Letters, 2009, 94, .	3.3	195
27	Structure and bulk modulus of M ₂ AlC (M=Ti, V, and Cr). Applied Physics Letters, 2003, 83, 899-901.	3.3	189
28	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. ACS Energy Letters, 2017, 2, 837-845.	17.4	187
29	TiO ₂ -Based Gas Sensor: A Possible Application to SO ₂ . ACS Applied Materials & Interfaces, 2013, 5, 8516-8522.	8.0	186
30	Potassium-Modified Mg(NH ₂) ₂ /2LiH System for Hydrogen Storage. Angewandte Chemie - International Edition, 2009, 48, 5828-5832.	13.8	181
31	Electronic structure of nanostructured ZnO from x-ray absorption and emission spectroscopy and the local density approximation. Physical Review B, 2004, 70, .	3.2	180
32	Ab initio calculations and experimental determination of the structure of Cr ₂ AlC. Solid State Communications, 2004, 130, 445-449.	1.9	179
33	Experimental and theoretical identification of a new high-pressure phase of silica. Nature, 1997, 388, 362-365.	27.8	177
34	Experimental and Theoretical Identification of a New High-Pressure TiO ₂ Polymorph. Physical Review Letters, 2001, 87, 275501.	7.8	175
35	Highly Sensitive and Selective Gas Detection Based on Silicene. Journal of Physical Chemistry C, 2015, 119, 16934-16940.	3.1	174
36	Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. Physical Review B, 2005, 71, .	3.2	173

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37	Ferromagnetism in Cu-doped ZnO from first-principles theory. <i>Physical Review B</i> , 2006, 74, .	3.2	166
38	Progress in supercapacitors: roles of two dimensional nanotubular materials. <i>Nanoscale Advances</i> , 2020, 2, 70-108.	4.6	164
39	Transverse Conductance of DNA Nucleotides in a Graphene Nanogap from First Principles. <i>Nano Letters</i> , 2011, 11, 1941-1945.	9.1	162
40	First-principles study of physisorption of nucleic acid bases on small-diameter carbon nanotubes. <i>Nanotechnology</i> , 2008, 19, 125701.	2.6	160
41	Symmetry Breaking Induced Bandgap in Epitaxial Graphene Layers on SiC. <i>Nano Letters</i> , 2008, 8, 4464-4468.	9.1	154
42	Elastic and optical properties of α - and β -Al ₂ O ₃ . <i>Physical Review B</i> , 1999, 59, 12777-12787.	3.2	152
43	Crystal structures of Ti, Zr, and Hf under compression: Theory. <i>Physical Review B</i> , 1993, 48, 16269-16279.	3.2	151
44	Li ⁺ ion conductivity and diffusion mechanism in α -Li ₃ N and β -Li ₃ N. <i>Energy and Environmental Science</i> , 2010, 3, 1524.	30.8	149
45	Toward the Realization of 2D Borophene Based Gas Sensor. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26869-26876.	3.1	148
46	Optical properties of the group-IVBrefractory metal compounds. <i>Physical Review B</i> , 1996, 54, 1673-1681.	3.2	147
47	Optical properties of Ti ₃ SiC ₂ and Ti ₄ AlN ₃ . <i>Applied Physics Letters</i> , 2008, 92, .	3.3	143
48	A possible mechanism for the emergence of an additional band gap due to a Ti-O-C bond in the TiO ₂ -graphene hybrid system for enhanced photodegradation of methylene blue under visible light. <i>RSC Advances</i> , 2014, 4, 59890-59901.	3.6	143
49	Borophane as a Benchmark of Graphene: A Potential 2D Material for Anode of Li and Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 16148-16158.	8.0	142
50	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. <i>Science Advances</i> , 2020, 6, eabb8097.	10.3	138
51	Superconductivity in Topological Insulator Sb ₂ Te ₃ Induced by Pressure. <i>Scientific Reports</i> , 2013, 3, 2016.	3.3	133
52	Electronic and optical properties of RuO ₂ and IrO ₂ . <i>Physical Review B</i> , 2006, 73, .	3.2	131
53	Encapsulating Trogtalite CoSe ₂ Nanobuds into BCN Nanotubes as High Storage Capacity Sodium Ion Battery Anodes. <i>Advanced Energy Materials</i> , 2019, 9, 1901778.	19.5	131
54	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se) Tj ETQq0 0 0,rgBT /Overlock 10 Tf	8.9	130

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55	Topological Insulating in GeTe Superlattice. Physical Review Letters, 2012, 109, 096802.	12.8	128
56	Core-shell nanostructures: perspectives towards drug delivery applications. Journal of Materials Chemistry B, 2020, 8, 8992-9027.	5.8	127
57	The curious case of two dimensional Si_2BN : A high-capacity battery anode material. Nano Energy, 2017, 41, 251-260.	16.0	121
58	High-pressure structural studies of hematite Fe_2O_3 . Physical Review B, 2002, 65, .	3.2	116
59	Optical properties of graphite from first-principles calculations. Physical Review B, 1997, 55, 4999-5005.	3.2	115
60	Structural Phase Transition of Vanadium at 69 GPa. Physical Review Letters, 2007, 98, 085502.	7.8	115
61	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. Journal of Catalysis, 2013, 299, 204-209.	6.2	115
62	A High-Pressure Structure in Curium Linked to Magnetism. Science, 2005, 309, 110-113.	12.6	112
63	Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure. Physical Review B, 2008, 77, .	3.2	112
64	N@Graphene : Highly Sensitive and Selective Gas Sensor. Journal of Physical Chemistry C, 2015, 119, 24827-24836.	3.1	112
65	Metal-Nonmetal Transition in the Boron Group Elements. Physical Review Letters, 2003, 90, 065701.	7.8	111
66	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride ($\text{g-C}_3\text{N}_4$) nanosheets under selected transition metal doping. International Journal of Hydrogen Energy, 2020, 45, 3035-3045.	7.1	110
67	Crystal structure and elastic-constant anomalies in the magnetic 3d transition metals. Physical Review B, 1994, 50, 5918-5927.	3.2	109
68	Quasiab initio molecular dynamic study of Cu melting. Physical Review B, 2000, 61, 3838-3844.	3.2	108
69	High-pressure and high-temperature synthesis of the cubic TiO_2 polymorph. Physical Review B, 2004, 70, .	3.2	108
70	Pressure-induced reversible amorphization and an amorphous-amorphous transition in $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase-change memory material. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10410-10414.	7.1	107
71	Room temperature ferromagnetism in pristine MgO thin films. Applied Physics Letters, 2010, 96, .	3.3	105
72	Structural properties of liquid Al_2O_3 : A molecular dynamics study. Physical Review E, 2000, 61, 2723-2729.	2.1	102

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91	Theoretical investigation of the solubility in $(M_xM_2^{1-x})AlC(M_1, M_2 = Ti, V, Cr)$. <i>Physical Review B</i> , 2003, 68, .	3.2	87
92	Electronic structure, magnetism, and Fermi surfaces of Gd and Tb. <i>Physical Review B</i> , 1994, 50, 5147-5154.	3.2	86
93	Theoretical Study of Electronic Transport through DNA Nucleotides in a Double-Functionalized Graphene Nanogap. <i>Journal of Physical Chemistry C</i> , 2013, 117, 15421-15428.	3.1	86
94	Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. <i>Applied Physics Letters</i> , 2016, 109, .	3.3	86
95	An oriented Ni-Co-MOF anchored on solution-free 1D CuO: a p-n heterojunction for supercapacitive energy storage. <i>Journal of Materials Chemistry A</i> , 2021, 9, 17790-17800.	10.3	86
96	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. <i>Journal of Materials Chemistry C</i> , 2019, 7, 12312-12320.	5.5	85
97	Anomalously enhanced superconductivity and lattice dynamics in transition metal carbides and nitrides. <i>Physical Review B</i> , 2005, 72, .	3.2	84
98	Light metal decorated graphdiyne nanosheets for reversible hydrogen storage. <i>Nanotechnology</i> , 2018, 29, 355401.	2.6	83
99	Theoretical and experimental study of the graphite 1s-x-ray absorption edges. <i>Physical Review B</i> , 1996, 54, 14396-14404.	3.2	82
100	Optical properties of monoclinic SnI ₂ from relativistic first-principles theory. <i>Physical Review B</i> , 1997, 56, 6851-6861.	3.2	82
101	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 17977-17991.	8.0	82
102	The role of Ge ₂ Sb ₂ Te ₅ in enhancing the performance of functional plasmonic devices. <i>Materials Today Physics</i> , 2020, 12, 100178.	6.0	82
103	Vacancy-mediated hydrogen desorption in NaAlH ₄ . <i>Physical Review B</i> , 2005, 72, .	3.2	81
104	General trend for pressurized superconducting hydrogen-dense materials. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 2793-2796.	7.1	81
105	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25256-25262.	3.1	81
106	Theoretical and experimental evidence of enhanced ferromagnetism in Ba and Mn cosubstituted BiFeO ₃ . <i>Applied Physics Letters</i> , 2010, 96, .	3.3	80
107	Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices. <i>Nanoscale</i> , 2016, 8, 11291-11305.	5.6	80
108	Electronic structure of phospho-olivines Li _x FePO ₄ (x=0,1) from soft-x-ray-absorption and -emission spectroscopies. <i>Journal of Chemical Physics</i> , 2005, 123, 184717.	3.0	79

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109	Noblest of All Metals Is Structurally Unstable at High Pressure. <i>Physical Review Letters</i> , 2007, 98, 045503.	7.8	79
110	Predicted High-Temperature Superconducting State in the Hydrogen-Dense Transition-Metal Hydride YH_3 at 40 ÅK and 17.7 ÅGPa. <i>Physical Review Letters</i> , 2009, 103, 077002.	7.8	79
111	Rhodium dihydride (RhH_2) with high volumetric hydrogen density. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 18618-18621.	7.1	78
112	Ultrahigh-pressure isostructural electronic transitions in hydrogen. <i>Nature</i> , 2019, 573, 558-562.	27.8	78
113	Efficient and selective sensing of nitrogen-containing gases by Si ₂ BN nanosheets under pristine and pre-oxidized conditions. <i>Applied Surface Science</i> , 2019, 469, 775-780.	6.1	78
114	Theoretical Investigation of High Pressure Phases of Carbon Dioxide. <i>Physical Review Letters</i> , 2000, 85, 1258-1261.	7.8	77
115	Borane Derivatives: A New Class of Super- and Hyperhalogens. <i>ChemPhysChem</i> , 2011, 12, 2423-2428.	2.1	77
116	Computational Evaluation of Lithium-Functionalized Carbon Nitride ($\text{g-C}_6\text{N}_8$) Monolayer as an Efficient Hydrogen Storage Material. <i>Journal of Physical Chemistry C</i> , 2016, 120, 25180-25188.	3.1	76
117	Polarization-dependent soft-x-ray absorption of highly oriented ZnO microrod arrays. <i>Journal of Physics Condensed Matter</i> , 2002, 14, 6969-6974.	1.8	74
118	Predicted Formation of Superconducting Platinum-Hydride Crystals under Pressure in the Presence of Molecular Hydrogen. <i>Physical Review Letters</i> , 2011, 107, 117002.	7.8	74
119	Ab initio calculations of the mechanical properties of Ti ₃ SiC ₂ . <i>Applied Physics Letters</i> , 2001, 79, 1450-1452.	3.3	73
120	Origin of Magnetic Anisotropy of Gd Metal. <i>Physical Review Letters</i> , 2003, 91, 157201.	7.8	73
121	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3456-3459.	3.1	73
122	Theoretical Confirmation of the High Pressure Simple Cubic Phase in Calcium. <i>Physical Review Letters</i> , 1995, 75, 3473-3476.	7.8	72
123	Theory of the ternary layered system Ti-Al-N. <i>Journal of Applied Physics</i> , 2002, 91, 9874.	2.5	72
124	Band gap engineering in huge-gap semiconductor SrZrO ₃ for visible-light photocatalysis. <i>International Journal of Hydrogen Energy</i> , 2014, 39, 2042-2048.	7.1	72
125	Melting of iron and other metals at earth's core conditions: A simplified computational approach. <i>Physical Review B</i> , 2001, 65, .	3.2	71
126	Anion-Doped NaTaO ₃ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013, 117, 22518-22524.	3.1	71

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127	Sensing Characteristics of Phosphorene Monolayers toward PH ₃ and AsH ₃ Gases upon the Introduction of Vacancy Defects. Journal of Physical Chemistry C, 2016, 120, 20428-20436.	3.1	71
128	2D-HfS ₂ as an efficient photocatalyst for water splitting. Catalysis Science and Technology, 2016, 6, 6605-6614.	4.1	71
129	Novel green phosphorene as a superior chemical gas sensing material. Journal of Hazardous Materials, 2021, 401, 123340.	12.4	71
130	Dynamic atmospheres and winds of cool luminous giants. Astronomy and Astrophysics, 2016, 594, A108.	5.1	71
131	Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes. Advanced Functional Materials, 2011, 21, 2674-2679.	14.9	70
132	Optical properties of Mg-doped VO ₂ : Absorption measurements and hybrid functional calculations. Applied Physics Letters, 2012, 101, .	3.3	70
133	<i>Ab initio</i> study of a 2D h-BAs monolayer: a promising anode material for alkali-metal ion batteries. Physical Chemistry Chemical Physics, 2019, 21, 18328-18337.	2.8	70
134	Integration of CuO nanosheets to Zn-Ni-Co oxide nanowire arrays for energy storage applications. Chemical Engineering Journal, 2021, 413, 127570.	12.7	70
135	Role of titanium in hydrogen desorption in crystalline sodium alanate. Applied Physics Letters, 2005, 86, 251913.	3.3	69
136	Structural and energetic analysis of the hydrogen storage materials LiNH_2 NaNH_2 Physical Review B, 2009, 79, .	3.2	69
137	Rationalizing the Hydrogen and Oxygen Evolution Reaction Activity of Two-Dimensional Hydrogenated Silicene and Germanene. ACS Applied Materials & Interfaces, 2016, 8, 1536-1544.	8.0	69
138	Adsorption mechanism of graphene-like ZnO monolayer towards CO ₂ molecules: enhanced CO ₂ capture. Nanotechnology, 2016, 27, 015502.	2.6	69
139	Reversible hydrogen storage properties of defect-engineered C_4N_4 nanosheets under ambient conditions. Car	10.3	69
140	Optical band-edge absorption of oxide compound SnO ₂ . Applied Surface Science, 2006, 252, 5361-5364.	6.1	68
141	The surface energy and stress of metals. Surface Science, 2018, 674, 51-68.	1.9	68
142	Peierls distortion mediated reversible phase transition in GeTe under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5948-5952.	7.1	67
143	Hybrid density functional study on SrTiO ₃ for visible light photocatalysis. International Journal of Hydrogen Energy, 2012, 37, 11611-11617.	7.1	67
144	Hierarchical Aerographite nano-microtubular tetrapodal networks based electrodes as lightweight supercapacitor. Nano Energy, 2017, 34, 570-577.	16.0	67

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145	Zn Metal Atom Doping on the Surface Plane of One-Dimensional NiMoO ₄ Nanorods with Improved Redox Chemistry. ACS Applied Materials & Interfaces, 2020, 12, 44815-44829.	8.0	67
146	CubicTiO ₂ as a potential light absorber in solar-energy conversion. Physical Review B, 2004, 70, .	3.2	66
147	Ionothermal Synthesis of High-Voltage <i>Alluaudite</i> Na _{2+2x} Fe _{2-x} (SO ₄) ₃ Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. ACS Applied Materials & Interfaces, 2016, 8, 6982-6991.	8.0	66
148	Sodium-intercalated bulk graphdiyne as an anode material for rechargeable batteries. Journal of Power Sources, 2017, 343, 354-363.	7.8	66
149	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. Applied Physics Letters, 2018, 112, .	3.3	66
150	Electronic structure of Ti ₃ SiC ₂ . Applied Physics Letters, 2000, 76, 2226-2228.	3.3	65
151	The structure of the metallic high-pressure Fe ₃ O ₄ polymorph: experimental and theoretical study. Journal of Physics Condensed Matter, 2003, 15, 7697-7706.	1.8	65
152	Beating the Miscibility Barrier between Iron Group Elements and Magnesium by High-Pressure Alloying. Physical Review Letters, 2005, 95, 245502.	7.8	65
153	Pressure-induced superconductivity in CaC ₂ . Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 9289-9294.	7.1	65
154	First principles design of Li functionalized hydrogenated h-BN nanosheet for hydrogen storage. International Journal of Hydrogen Energy, 2016, 41, 14437-14446.	7.1	65
155	Graphenylene Monolayers Doped with Alkali or Alkaline Earth Metals: Promising Materials for Clean Energy Storage. Journal of Physical Chemistry C, 2017, 121, 14393-14400.	3.1	65
156	Non-transition-metal doped diluted magnetic semiconductors. Applied Physics Letters, 2009, 94, .	3.3	64
157	Molecular Simulation for Gas Adsorption at NiO (100) Surface. ACS Applied Materials & Interfaces, 2012, 4, 5691-5697.	8.0	64
158	Optical properties of PdO and PtO. Physical Review B, 1994, 50, 2128-2132.	3.2	63
159	Selective decoration of nitrogenated holey graphene (C ₂ N) with titanium clusters for enhanced hydrogen storage application. International Journal of Hydrogen Energy, 2021, 46, 7371-7380.	7.1	63
160	Balanced crystal orbital overlap population—a tool for analysing chemical bonds in solids. Journal of Physics Condensed Matter, 2003, 15, 7751-7761.	1.8	62
161	Superconductivity in Strong Spin Orbital Coupling Compound Sb ₂ Se ₃ . Scientific Reports, 2014, 4, 6679.	3.3	62
162	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. Sustainable Energy and Fuels, 2020, 4, 2363-2369.	4.9	62

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163	Designing strategies to tune reduction potential of organic molecules for sustainable high capacity battery application. Journal of Materials Chemistry A, 2017, 5, 4430-4454.	10.3	61
164	Electronic Structure, Optical Properties, and Photocatalytic Activities of LaFeO_3 - NaTaO_3 Solid Solution. Journal of Physical Chemistry C, 2012, 116, 22767-22773.	3.1	60
165	Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries. Journal of Power Sources, 2021, 485, 229318.	7.8	60
166	Electronic structure investigation of Ti_3AlC_2 , Ti_3SiC_2 , and Ti_3GeC_2 by soft x-ray emission spectroscopy. Physical Review B, 2005, 72, .	3.2	59
167	Electronic structure and chemical bonding in Ti_2AlC investigated by soft x-ray emission spectroscopy. Physical Review B, 2006, 74, .	3.2	59
168	Tunable Assembly of sp^3 Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. Advanced Functional Materials, 2013, 23, 5846-5853.	14.9	59
169	Dynamical stability of body center cubic iron at the Earth's core conditions. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9962-9964.	7.1	58
170	Electronic structure of graphite: Effect of hydrostatic pressure. Physical Review B, 1995, 51, 4813-4819.	3.2	57
171	High-pressure study of titanium carbide. Journal of Alloys and Compounds, 1999, 289, 24-27.	5.5	57
172	Structure of the GeSbTe phase-change materials studied by theory and experiment. Solid State Communications, 2007, 143, 240-244.	1.9	57
173	Study of Ti_2SC under compression up to 47GPa. Journal of Alloys and Compounds, 2008, 448, L1-L4.	5.5	57
174	Effective electronic masses in wurtzite and zinc-blende GaN and AlN. Journal of Crystal Growth, 2001, 231, 397-406.	1.5	56
175	First-principle calculations of optical properties of wurtzite AlN and GaN. Journal of Crystal Growth, 2001, 231, 407-414.	1.5	56
176	Adsorption characteristics of DNA nucleobases, aromatic amino acids and heterocyclic molecules on silicene and germanene monolayers. Sensors and Actuators B: Chemical, 2018, 255, 2713-2720.	7.8	56
177	Thermoelastic properties of random alloys from first-principles theory. Physical Review B, 2006, 73, .	3.2	55
178	Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. Applied Physics Letters, 2012, 101, .	3.3	55
179	On the semiconducting state and structural properties of YH ₃ from first principles theory. Applied Physics Letters, 1997, 71, 3498-3500.	3.3	54
180	Melting and liquid structure of aluminum oxide using a molecular-dynamics simulation. Physical Review E, 1998, 57, 1673-1676.	2.1	54

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181	Molecular dynamics of LiF melting. Physical Review B, 2000, 61, 11928-11935.	3.2	54
182	Electron-phonon coupling of $\text{f}^{\pm\text{g}}$ Gaboron. Physical Review B, 2004, 70, .	3.2	54
183	High-Pressure Melting of MgSiO_3 . Physical Review Letters, 2005, 94, 195701.	7.8	54
184	Band gap engineering in BiNbO_4 for visible-light photocatalysis. Applied Physics Letters, 2012, 100, 182102.	3.3	54
185	Reduction of shock-wave data with mean-field potential approach. Journal of Applied Physics, 2002, 92, 6616-6620.	2.5	53
186	Sensing propensity of a defected graphene sheet towards CO , H_2 and NO_2 . Nanotechnology, 2014, 25, 325501.	2.6	53
187	Enriching physisorption of H_2 and NH_3 gases on a graphene sheet by doping with Li adatoms. Physical Chemistry Chemical Physics, 2014, 16, 8100-8105.	2.8	53
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