Chandra Veer Singh

List of Publications by Year
in descending order

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162 papers	7,141 citations	47006 47 h-index	69250 77 g-index
165 all docs	165 docs citations	165 times ranked	8324 citing authors

#	Article	IF	Citations
1	Determining the limiting factor of the electrochemical stability window for PEO-based solid polymer electrolytes: main chain or terminal â€“OH group?. Energy and Environmental Science, 2020, 13, 1318-1325.	30.8	342
2	Phosphorene as a Polysulfide Immobilizer and Catalyst in Highâ€Performance Lithiumâ€“Sulfur Batteries. Advanced Materials, 2017, 29, 1602734.	21.0	289
3	Vertically Oriented Arrays of ReS₂ Nanosheets for Electrochemical Energy Storage and Electrocatalysis. Nano Letters, 2016, 16, 3780-3787.	9.1	241
4	Photoexcited Surface Frustrated Lewis Pairs for Heterogeneous Photocatalytic CO₂ Reduction. Journal of the American Chemical Society, 2016, 138, 1206-1214.	13.7	210
5	Illuminating CO₂ reduction on frustrated Lewis pair surfaces: investigating the role of surface hydroxides and oxygen vacancies on nanocrystalline In₂O_{3â^'x}(OH)_y. Physical Chemistry Chemical Physics, 2015, 17, 14623-14635.	2.8	186
6	Ultrahigh Storage and Fast Diffusion of Na and K in Blue Phosphorene Anodes. ACS Applied Materials & Interfaces, 2018, 10, 8630-8639.	8.0	143
7	Mechanochemistry for ammonia synthesis under mild conditions. Nature Nanotechnology, 2021, 16, 325-330.	31.5	141
8	High strength measurement of monolayer graphene oxide. Carbon, 2015, 81, 497-504.	10.3	138
9	A Foldable Lithiumâ€“Sulfur Battery. ACS Nano, 2015, 9, 11342-11350.	14.6	125
10	Catalytic CO2 reduction by palladium-decorated siliconâ€“hydride nanosheets. Nature Catalysis, 2019, 2, 46-54.	34.4	116
11	Adsorption of Metallic, Metalloidic, and Nonmetallic Adatoms on Two-Dimensional C₃N. Journal of Physical Chemistry C, 2017, 121, 18575-18583.	3.1	111
12	Fatigue of graphene. Nature Materials, 2020, 19, 405-411.	27.5	110
13	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. Nanoscale, 2018, 10, 3759-3768.	5.6	109
14	Amorphous TiO2 as a Photocatalyst for Hydrogen Production: A DFT Study of Structural and Electronic Properties. Energy Procedia, 2012, 29, 291-299.	1.8	108
15	Adsorption and Dissociation of H₂O on Monolayered MoS₂ Edges: Energetics and Mechanism from ab Initio Simulations. Journal of Physical Chemistry C, 2015, 119, 6518-6529.	3.1	107
16	Mechanical properties of monolayer penta-graphene and phagraphene: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 26736-26742.	2.8	106
17	Consequences of Surface Oxophilicity of Ni, Ni-Co, and Co Clusters on Methane Activation. Journal of the American Chemical Society, 2017, 139, 6928-6945.	13.7	104
18	Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO₂ with High Activity and Tailored Selectivity. Advanced Science, 2017, 4, 1700252.	11.2	97

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19	Defect engineering of graphene for effective hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 4981-4995.	7.1	96
20	Development of constitutive material model of 3D printed structure via FDM. Materials Today Communications, 2018, 15, 143-152.	1.9	94
21	Heterogeneous reduction of carbon dioxide by hydride-terminated silicon nanocrystals. Nature Communications, 2016, 7, 12553.	12.8	93
22	2D Hydrogenated graphene-like borophene as a high capacity anode material for improved Li/Na ion batteries: A first principles study. Materials Today Energy, 2018, 8, 22-28.	4.7	93
23	Adsorption and Diffusion of Lithium and Sodium on Defective Rhenium Disulfide: A First Principles Study. ACS Applied Materials & Interfaces, 2018, 10, 5373-5384.	8.0	92
24	Band Engineering of Carbon Nitride Monolayers by N-Type, P-Type, and Isoelectronic Doping for Photocatalytic Applications. ACS Applied Materials & Interfaces, 2018, 10, 11143-11151.	8.0	92
25	Tailoring Surface Frustrated Lewis Pairs of In₂O_{3â˜'}_x(OH)_y for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO₂ by Isomorphous Substitution of In³⁺ with Bi³⁺. Advanced Science, 2018, 5, 1700732.	11.2	91
26	Interface Engineering of Co/CoMoN/NF Heterostructures for Highâ€Performance Electrochemical Overall Water Splitting. Advanced Science, 2022, 9, e2105313.	11.2	90
27	Carrier dynamics and the role of surface defects: Designing a photocatalyst for gas-phase CO ₂ reduction. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8011-E8020.	7.1	89
28	Evolution of ply cracks in multidirectional composite laminates. International Journal of Solids and Structures, 2010, 47, 1338-1349.	2.7	86
29	A synergistic damage mechanics approach for composite laminates with matrix cracks in multiple orientations. Mechanics of Materials, 2009, 41, 954-968.	3.2	85
30	Enhanced photothermal reduction of gaseous CO₂ over silicon photonic crystal supported ruthenium at ambient temperature. Energy and Environmental Science, 2018, 11, 3443-3451.	30.8	83
31	Neural Network-Assisted Development of High-Entropy Alloy Catalysts: Decoupling Ligand and Coordination Effects. Matter, 2020, 3, 1318-1333.	10.0	83
32	Mechanisms of Guinierâ€“Preston zone hardening in the athermal limit. Acta Materialia, 2010, 58, 5797-5805.	7.9	81
33	Surface Analogues of Molecular Frustrated Lewis Pairs in Heterogeneous CO₂ Hydrogenation Catalysis. ACS Catalysis, 2016, 6, 5764-5770.	11.2	80
34	Metadynamics-Biased ab Initio Molecular Dynamics Study of Heterogeneous CO₂ Reduction via Surface Frustrated Lewis Pairs. ACS Catalysis, 2016, 6, 7109-7117.	11.2	78
35	Nonlinear fracture toughness measurement and crack propagation resistance of functionalized graphene multilayers. Science Advances, 2018, 4, eaao7202.	10.3	72
36	Adsorption and diffusion of lithium polysulfides over blue phosphorene for Liâ€“S batteries. Nanoscale, 2018, 10, 21335-21352.	5.6	69

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37	Interfacial Shear Strength of Multilayer Graphene Oxide Films. ACS Nano, 2016, 10, 1939-1947.	14.6	64
38	Hydrogen storage in Li, Na and Ca decorated and defective borophene: a first principles study. RSC Advances, 2018, 8, 20748-20757.	3.6	64
39	Deciphering Interfacial Chemical and Electrochemical Reactions of Sulfideâ€Based Allâ€Solidâ€State Batteries. Advanced Energy Materials, 2021, 11, 2100210.	19.5	63
40	Analysis of multiple off-axis ply cracks in composite laminates. International Journal of Solids and Structures, 2008, 45, 4574-4589.	2.7	61
41	Strengthening in Graphene Oxide Nanosheets: Bridging the Gap between Interplanar and Intraplanar Fracture. Nano Letters, 2015, 15, 6528-6534.	9.1	61
42	Atomistic simulations of dislocationâ€“precipitate interactions emphasize importance of cross-slip. Scripta Materialia, 2011, 64, 398-401.	5.2	58
43	Highly Efficient Ambient Temperature CO₂ Photomethanation Catalyzed by Nanostructured RuO₂ on Silicon Photonic Crystal Support. Advanced Energy Materials, 2018, 8, 1702277.	19.5	58
44	A representative volume element based on translational symmetries for FE analysis of cracked laminates with two arrays of cracks. International Journal of Solids and Structures, 2009, 46, 1793-1804.	2.7	56
45	A first principles study of hydrogen storage inÂlithium decorated defective phosphorene. International Journal of Hydrogen Energy, 2017, 42, 23018-23027.	7.1	56
46	Theoretical Investigation: 2D N-Graphdiyne Nanosheets as Promising Anode Materials for Li/Na Rechargeable Storage Devices. ACS Applied Nano Materials, 2019, 2, 127-135.	5.0	56
47	A first principles study of hydrogen storage on lithium decorated two dimensional carbon allotropes. International Journal of Hydrogen Energy, 2015, 40, 6128-6136.	7.1	53
48	Computational screening of homo and hetero transition metal dimer catalysts for reduction of CO₂ to C₂ products with high activity and low limiting potential. Journal of Materials Chemistry A, 2020, 8, 21241-21254.	10.3	51
49	Machine-learning-accelerated discovery of single-atom catalysts based on bidirectional activation mechanism. Chem Catalysis, 2021, 1, 183-195.	6.1	50
50	Predicting evolution of ply cracks in composite laminates subjected toÂbiaxial loading. Composites Part B: Engineering, 2015, 75, 264-273.	12.0	48
51	A triple atom catalyst with ultrahigh loading potential for nitrogen electrochemical reduction. Journal of Materials Chemistry A, 2020, 8, 15086-15093.	10.3	48
52	Development of a physics-based multi-scale progressive damage model for assessing the durability of wind turbine blades. Composite Structures, 2016, 141, 50-62.	5.8	46
53	Friction of Ti₃C₂T_x MXenes. Nano Letters, 2022, 22, 3356-3363.	9.1	46
54	Analysis of the Material Behavior of 3D Printed Laminates Via FFF. Experimental Mechanics, 2019, 59, 871-881.	2.0	45

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55	A molecular dynamic simulation on the factors influencing the fluidity of molten coke ash during alkalization with K2O and Na2O. Chemical Engineering Journal, 2017, 313, 1184-1193.	12.7	44
56	Carbon ene-yne graphyne monolayer as an outstanding anode material for Li/Na ion batteries. Applied Materials Today, 2018, 10, 115-121.	4.3	44
57	Toughening of graphene-based polymer nanocomposites via tuning chemical functionalization. Composites Science and Technology, 2020, 194, 108140.	7.8	44
58	Uncertainty analysis and estimation of robust AIREBO parameters for graphene. Carbon, 2019, 142, 300-310.	10.3	43
59	Tailoring lattice strain in ultra-fine high-entropy alloys for active and stable methanol oxidation. Science China Materials, 2021, 64, 2454-2466.	6.3	43
60	A synergistic damage mechanics based multiscale model for composite laminates subjected to multiaxial strains. Mechanics of Materials, 2015, 83, 72-89.	3.2	42
61	Solar grade silicon production: A review of kinetic, thermodynamic and fluid dynamics based continuum scale modeling. Renewable and Sustainable Energy Reviews, 2017, 78, 1288-1314.	16.4	40
62	Transition metalâ€“N₄ embedded black phosphorus carbide as a high-performance bifunctional electrocatalyst for ORR/OER. Nanoscale, 2020, 12, 18721-18732.	5.6	39
63	A synergistic damage mechanics approach to mechanical response of composite laminates with ply cracks. Journal of Composite Materials, 2013, 47, 2475-2501.	2.4	38
64	Twoâ€dimensional boron as an impressive lithiumâ€sulphur battery cathode material. Energy Storage Materials, 2018, 13, 80-87.	18.0	38
65	Importance of quadratic dispersion in acoustic flexural phonons for thermal transport of two-dimensional materials. Physical Review B, 2021, 103, .	3.2	38
66	Competing twinning mechanisms in body-centered cubic metallic nanowires. Scripta Materialia, 2016, 113, 214-217.	5.2	37
67	Prediction of ply crack evolution and stiffness degradation in multidirectional symmetric laminates under multiaxial stress states. Composites Part B: Engineering, 2018, 133, 53-67.	12.0	37
68	Harnessing atomistic simulations to predict the rate at which dislocations overcome obstacles. Journal of the Mechanics and Physics of Solids, 2016, 90, 203-214.	4.8	36
69	A van der Waals density functional theory comparison of metal decorated graphene systems for hydrogen adsorption. Journal of Applied Physics, 2014, 115, 224301.	2.5	35
70	An Atomistic-Based Hierarchical Multiscale Examination of Age Hardening in an Al-Cu Alloy. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 2625-2644.	2.2	34
71	Insights on the dual role of two-dimensional materials as catalysts and supports for energy and environmental catalysis. Journal of Materials Chemistry A, 2021, 9, 2018-2042.	10.3	34
72	New insights into the structure-nonlinear mechanical property relations for graphene allotropes. Carbon, 2016, 110, 443-457.	10.3	32

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73	Effect of doping on electronic structure and photocatalytic behavior of amorphous TiO2. Journal of Physics Condensed Matter, 2013, 25, 475501.	1.8	30
74	The ideal strength of two-dimensional stanene may reach or exceed the Griffith strength estimate. Nanoscale, 2017, 9, 7055-7062.	5.6	29
75	Assessing progressive failure in long wind turbine blades under quasi-static and cyclic loads. Renewable Energy, 2018, 119, 754-766.	8.9	29
76	Predicting aggregation energy for single atom bimetallic catalysts on clean and O* adsorbed surfaces through machine learning models. Catalysis Science and Technology, 2020, 10, 86-98.	4.1	29
77	Temperature dependence of grain boundary excess free volume. Scripta Materialia, 2020, 178, 71-76.	5.2	29
78	Phosphorene as a Catalyst for Highly Efficient Nonaqueous Liâ€“Air Batteries. ACS Applied Materials & Interfaces, 2019, 11, 499-510.	8.0	27
79	Understanding the Independent and Interdependent Role of Water and Oxidation on the Tribology of Ultrathin Molybdenum Disulfide (MoS₂). Advanced Materials Interfaces, 2019, 6, 1901246.	3.7	26
80	Electrolyte-Phobic Surface for the Next-Generation Nanostructured Battery Electrodes. Nano Letters, 2020, 20, 7455-7462.	9.1	25
81	A DFT +Ustudy of (Rh, Nb)-codoped rutile TiO₂. Journal of Physics Condensed Matter, 2013, 25, 085501.	1.8	23
82	Effects of topological point reconstructions on the fracture strength and deformation mechanisms of graphene. Computational Materials Science, 2015, 97, 172-180.	3.0	23
83	Atomistic Origins of Ductility Enhancement in Metal Oxide Coated Silicon Nanowires for Liâ€ion Battery Anodes. Advanced Materials Interfaces, 2017, 4, 1700920.	3.7	23
84	Structurally ordered highâ€entropy intermetallic nanoparticles with enhanced Câ€“C bond cleavage for ethanol oxidation. SmartMat, 2023, 4, .	10.7	23
85	Role of graphene in enhancing the mechanical properties of TiO₂/graphene heterostructures. Nanoscale, 2017, 9, 11678-11684.	5.6	22
86	Effect of lattice stacking orientation and local thickness variation on the mechanical behavior of few layer graphene oxide. Carbon, 2018, 136, 168-175.	10.3	21
87	Friction of magnetene, a nonâ€“van der Waals 2D material. Science Advances, 2021, 7, eabk2041.	10.3	21
88	Development and implementation of a multi-scale model for matrix micro-cracking prediction in composite structures subjected to low velocity impact. Composites Part B: Engineering, 2019, 168, 140-151.	12.0	20
89	Fastâ€Charging Halideâ€Based Allâ€Solidâ€State Batteries by Manipulation of Current Collector Interface. Advanced Functional Materials, 2022, 32, .	14.9	20
90	A kinematic study of energy barriers for crack formation in graphene tilt boundaries. Journal of Applied Physics, 2014, 115, .	2.5	19

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91	How does mass transfer influence electrochemical carbon dioxide reduction reaction? A case study of Ni molecular catalyst supported on carbon. Chemical Communications, 2021, 57, 1384-1387.	4.1	18
92	Mechanical Size Effect of Freestanding Nanoconfined Polymer Films. Macromolecules, 2022, 55, 1248-1259.	4.8	18
93	Self-Trapped Charge Carriers in Defected Amorphous TiO₂. Journal of Physical Chemistry C, 2016, 120, 27910-27916.	3.1	17
94	Molecular Dynamics Investigation on Coke Ash Behavior in the High-Temperature Zones of a Blast Furnace: Influence of Alkalis. Energy & Fuels, 2017, 31, 13466-13474.	5.1	17
95	Phase Evolution of a Prenucleator for Fast Li Nucleation in Allâ€Solidâ€State Lithium Batteries. Advanced Energy Materials, 2020, 10, 2001191.	19.5	17
96	A first-principles study of the relationship between modulus and ideal strength of single-layer, transition metal dichalcogenides. Materials Advances, 2021, 2, 6631-6640.	5.4	17
97	Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. Physical Chemistry Chemical Physics, 2020, 22, 22758-22767.	2.8	15
98	Two-Dimensional Graphdiyne-Confined Platinum Catalyst for Hydrogen Evolution and Oxygen Reduction Reactions. ACS Applied Materials & Interfaces, 2021, 13, 47541-47548.	8.0	15
99	Molecular adsorption and surface formation reactions of HCl, H2 and chlorosilanes on Si(100)-c(4â€Ã—â€2) with applications for high purity silicon production. Applied Surface Science, 2019, 475, 124-134.	6.1	14
100	Fatigue resistance of atomically thin graphene oxide. Carbon, 2021, 183, 780-788.	10.3	14
101	Deformation behavior of a NiCo multilayer with a modulated grain size distribution. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2015, 641, 305-314.	5.6	13
102	Role of niobium and oxygen concentration on glass forming ability and crystallization behavior of Zr-Ni-Al-Cu-Nb bulk metallic glasses with low copper concentration. Journal of Non-Crystalline Solids, 2016, 445-446, 88-94.	3.1	13
103	Critical stiffness damage envelopes for multidirectional laminated structures under multiaxial loading conditions. Materials and Design, 2016, 91, 218-229.	7.0	13
104	Structureâ€Ðependent Wear and Shear Mechanics of Nanostructured MoS₂ Coatings. Advanced Materials Interfaces, 2020, 7, 1901870.	3.7	13
105	Microtissue Engineering Root Dentin with Photodynamically Cross-linked Nanoparticles Improves Fatigue Resistance of Endodontically Treated Teeth. Journal of Endodontics, 2020, 46, 668-674.	3.1	13
106	Fundamental Insights into Electrical and Transport Properties of Chloroaluminate Ionic Liquids for Aluminum-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 15145-15154.	3.1	13
107	Size effects in strengthening of NiCo multilayers with modulated microstructures. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 771, 138581.	5.6	12
108	Dramatic improvement in the performance of graphene as Li/Na battery anodes with suitable electrolytic solvents. Carbon, 2020, 161, 570-576.	10.3	12

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109	Strength of graphene with curvilinear grain boundaries. Carbon, 2020, 158, 808-817.	10.3	11
110	Machine learned interatomic potentials using random features. Npj Computational Materials, 2022, 8, .	8.7	11
111	Two-dimensional square metal organic framework as promising cathode material for lithium-sulfur battery with high theoretical energy density. Journal of Colloid and Interface Science, 2022, 613, 435-446.	9.4	11
112	Interplay between Thermal Stress and Interface Binding on Fracture of WS₂ Monolayer with Triangular Voids. ACS Applied Materials & Interfaces, 2022, 14, 16876-16884.	8.0	10
113	Investigating the atomic level influencing factors of glass forming ability in NiAl and CuZr metallic glasses. Journal of Chemical Physics, 2015, 143, 114509.	3.0	9
114	First Principles Investigation of HCl, H₂, and Chlorosilane Adsorption on Cu₃Si Surfaces with Applications for Polysilicon Production. Journal of Physical Chemistry C, 2018, 122, 20252-20260.	3.1	9
115	Kinetics of annealing-induced detwinning in chemical vapor deposited nickel. Acta Materialia, 2019, 178, 263-274.	7.9	9
116	Effect of He on the Order-Disorder Transition in Ni3Al under Irradiation. Physical Review Letters, 2020, 124, 075901.	7.8	9
117	Anisotropic phonon thermal transport in nitrophosphorene monolayer. Physical Review Materials, 2021, 5, .	2.4	9
118	Development of a synergistic damage mechanics model to predict evolution of ply cracking and stiffness changes in multidirectional composite laminates under creep. International Journal of Damage Mechanics, 2016, 25, 1060-1078.	4.2	8
119	Uncertainty and sensitivity analysis of mechanical and thermal properties computed through Embedded Atom Method potential. Computational Materials Science, 2019, 166, 30-41.	3.0	8
120	Elastomer-like deformation in high-Poisson's-ratio graphene allotropes may allow tensile strengths beyond theoretical cohesive strength limits. Carbon, 2019, 143, 752-761.	10.3	8
121	Interfacial Interactions and Tribological Behavior of Metal-Oxide/2D-Material Contacts. Tribology Letters, 2021, 69, 1.	2.6	8
122	High-throughput and machine-learning accelerated design of high entropy alloy catalysts. Trends in Chemistry, 2022, 4, 577-579.	8.5	8
123	Solar Fuels: Highly Efficient Ambient Temperature CO₂ Photomethanation Catalyzed by Nanostructured RuO₂ on Silicon Photonic Crystal Support (Adv. Energy Mater. 9/2018). Advanced Energy Materials, 2018, 8, 1870041.	19.5	7
124	Performance Analysis of Composite Helicopter Blade Using Synergistic Damage Mechanics Approach. AIAA Journal, 2020, 58, 968-976.	2.6	7
125	Machine learning-enabled band gap prediction of monolayer transition metal chalcogenide alloys. Physical Chemistry Chemical Physics, 2022, 24, 4653-4665.	2.8	7
126	High-Strength, Microporous, Two-Dimensional Polymer Thin Films with Rigid Benzoxazole Linkage. ACS Applied Materials & Interfaces, 2022, 14, 1861-1873.	8.0	7

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127	Short-range structural origins of serration events in metallic glasses. Journal of Alloys and Compounds, 2019, 787, 840-850.	5.5	6
128	Defect evolution behaviors from single sulfur point vacancies to line vacancies in monolayer molybdenum disulfide. Physical Chemistry Chemical Physics, 2021, 23, 19525-19536.	2.8	6
129	Identification of Tetramers in Silver Films Grown on the Si(001) Surface at Room Temperature. Journal of Physical Chemistry Letters, 2018, 9, 6275-6279.	4.6	5
130	Time-dependent damage analysis for viscoelastic-viscoplastic structural laminates under biaxial loading. Composite Structures, 2018, 203, 60-70.	5.8	5
131	Deformation behavior of BCC tantalum nanolayered composites with modulated layer thicknesses. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2019, 761, 138037.	5.6	5
132	Synergistic vacancy defects and mechanical strain for the modulation of the mechanical, electronic and optical properties of monolayer tungsten disulfide. Physical Chemistry Chemical Physics, 2021, 23, 6298-6308.	2.8	5
133	Bias dependence and defect analysis of Bi on Si(111) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>Ã—</mml:mo> width="4pt" /><mml:mi>Î²</mml:mi></mml:mrow></mml:math> -phase. Physical Review B, 2021, 103, .	3.2	5
134	Neural evolution structure generation: High entropy alloys. Journal of Chemical Physics, 2021, 155, 044102.	3.0	5
135	Quantum well states and sizable Rashba splitting on Pb induced Î±-phase Bi/Si(111) surface reconstruction. Nanoscale, 2021, 13, 16622-16628.	5.6	5
136	Eggshell-like MoS₂ Nanostructures with Negative Curvature and Stepped Faces for Efficient Hydrogen Evolution Reactions. ACS Applied Nano Materials, 2021, 4, 14086-14093.	5.0	5
137	Mechanical reliability of monolayer MoS2 and WSe2. Matter, 2022, 5, 2975-2989.	10.0	5
138	Multiscale Modeling for Damage Analysis. , 2008, , 529-578.		4
139	Effect of matrix cracks and delamination on extension-twist coupling of thin pretwisted composite strips. Composite Structures, 2017, 180, 234-250.	5.8	4
140	How Silver Grows on the Silicon (001) Surface: A Theoretical and Experimental Investigation. ACS Applied Electronic Materials, 2019, 1, 122-131.	4.3	4
141	Insights into oxygen activation on metal clusters for catalyst design. Journal of Materials Chemistry A, 2021, 9, 11726-11733.	10.3	4
142	Thermoconformational Behavior of Cellulose Nanofiber Films as a Device Substrate and Their Superior Flexibility and Durability to Glass. ACS Applied Materials & Interfaces, 2021, 13, 40853-40862.	8.0	4
143	Mechanistic Origin of Orientation-Dependent Substructure Evolution in Aluminum and Aluminum-Magnesium Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2022, 53, 2689-2707.	2.2	4
144	Solar Fuels: Tailoring Surface Frustrated Lewis Pairs of In₂O_{3â^'}_x(OH)_y for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO₂ by Isomorphous Substitution of In³⁺ with Bi³⁺ (Adv. Sci. 6/2018). Advanced Science, 2018, 5, 1870034.	11.2	3

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145	Atomic structure of Ni-Nb-Y amorphous alloys and water-surface adsorption characteristics. Computational Materials Science, 2019, 169, 109095.	3.0	3
146	Damage Mechanics of Composite Laminates with Transverse Matrix Cracks in Multiple Orientations. , 2007, , .		2
147	A Practical Investigation of the Production of Zr-Cu-Al-Ni Bulk Metallic Glasses by Arc Melting and Suction Casting. Materials Transactions, 2015, 56, 1834-1841.	1.2	2
148	Photothermal Catalysis: Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO₂ with High Activity and Tailored Selectivity (Adv. Sci. 10/2017). Advanced Science, 2017, 4, .	11.2	2
149	A molecular dynamics study of dislocation ejection and shear coupling associated with incoherent twin boundary migration. Materialia, 2021, 16, 101111.	2.7	2
150	Progressive Failure Analysis of Polymer Composites Using a Synergistic Damage Mechanics Methodology. , 2014, , 147-155.		2
151	Extraordinary lattice thermal conductivity of gold sulfide monolayers. Nanoscale Advances, 2022, 4, 2873-2883.	4.6	2
152	Automatically Capturing Key Features for Predicting Superionic Conductivity of Solid-State Electrolytes Using a Neural Network. ACS Applied Energy Materials, 2022, 5, 8042-8048.	5.1	2
153	Atomistic study of crack-tip plasticity in precipitation hardened monocrystalline aluminum. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 065009.	2.0	1
154	Hindered surface diffusion of bonded molecular clusters mediated by surface defects. Physical Review Materials, 2020, 4, .	2.4	1
155	Chemical and molecular structure transformations in atomistic conformation of cellulose nanofibers under thermal environment. Npj Materials Degradation, 2022, 6, .	5.8	1
156	Macro-damage mechanics. , 0, , 134-178.		0
157	Damage progression. , 0, , 179-236.		0
158	Development of a Synergistic Damage Mechanics-Based Model for Predicting Multiaxial Effects in Progressive Failure of Composite Structures. , 2014, , .		0
159	Failure mechanisms in thin-walled nanocrystalline cylinders under uniaxial compression. Acta Materialia, 2015, 86, 157-168.	7.9	0
160	A fast mollified impulse method for biomolecular atomistic simulations. Journal of Computational Physics, 2017, 333, 180-198.	3.8	0
161	2.7 Micromechanics of Damage Evolution in Laminates. , 2018, , 118-147.		0
162	Compression-induced resistance of singlet oxygen dissociation on phosphorene. Physical Review Materials, 2020, 4, .	2.4	0