Chandra Veer Singh

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Structurally ordered highâ€entropy intermetallic nanoparticles with enhanced C–C bond cleavage for ethanol oxidation. SmartMat, 2023, 4, .	10.7	23
2	Machine learning-enabled band gap prediction of monolayer transition metal chalcogenide alloys. Physical Chemistry Chemical Physics, 2022, 24, 4653-4665.	2.8	7
3	High-Strength, Microporous, Two-Dimensional Polymer Thin Films with Rigid Benzoxazole Linkage. ACS Applied Materials & Interfaces, 2022, 14, 1861-1873.	8.0	7
4	Machine learned interatomic potentials using random features. Npj Computational Materials, 2022, 8, .	8.7	11
5	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
6	Mechanical Size Effect of Freestanding Nanoconfined Polymer Films. Macromolecules, 2022, 55, 1248-1259.	4.8	18
7	Interface Engineering of Co/CoMoN/NF Heterostructures for Highâ€Performance Electrochemical Overall Water Splitting. Advanced Science, 2022, 9, e2105313.	11.2	90
8	Chemical and molecular structure transformations in atomistic conformation of cellulose nanofibers under thermal environment. Npj Materials Degradation, 2022, 6, .	5.8	1
9	Fastâ€Charging Halideâ€Based Allâ€Solidâ€State Batteries by Manipulation of Current Collector Interface. Advanced Functional Materials, 2022, 32, .	14.9	20
10	Interplay between Thermal Stress and Interface Binding on Fracture of WS ₂ Monolayer with Triangular Voids. ACS Applied Materials & Interfaces, 2022, 14, 16876-16884.	8.0	10
11	Friction of Ti ₃ C ₂ T _{<i>x</i>} MXenes. Nano Letters, 2022, 22, 3356-3363.	9.1	46
12	High-throughput and machine-learning accelerated design of high entropy alloy catalysts. Trends in Chemistry, 2022, 4, 577-579.	8.5	8
13	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
14	Extraordinary lattice thermal conductivity of gold sulfide monolayers. Nanoscale Advances, 2022, 4, 2873-2883.	4.6	2
15	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
16	Mechanical reliability of monolayer MoS2 and WSe2. Matter, 2022, 5, 2975-2989.	10.0	5
17	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
18	Mechanochemistry for ammonia synthesis under mild conditions. Nature Nanotechnology, 2021, 16, 325-330.	31.5	141

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19	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
20	Insights into oxygen activation on metal clusters for catalyst design. Journal of Materials Chemistry A, 2021, 9, 11726-11733.	10.3	4
21	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
22	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
23	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
24	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>width="4pt" /><mml:mi>î²</mml:mi></mml:msqrt></mml:mrow> -phase. Physical Review B, 2021, 103, .</mml:math 	m sqz t> <m< td=""><td>ımatmo>×<</td></m<>	ımatmo>×<
25	Anisotropic phonon thermal transport in nitrophosphorene monolayer. Physical Review Materials, 2021, 5, .	2.4	9
26	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
27	Deciphering Interfacial Chemical and Electrochemical Reactions of Sulfideâ€Based Allâ€Solidâ€State Batteries. Advanced Energy Materials, 2021, 11, 2100210.	19.5	63
28	A molecular dynamics study of dislocation ejection and shear coupling associated with incoherent twin boundary migration. Materialia, 2021, 16, 101111.	2.7	2
29	Machine-learning-accelerated discovery of single-atom catalysts based on bidirectional activation mechanism. Chem Catalysis, 2021, 1, 183-195.	6.1	50
30	Interfacial Interactions and Tribological Behavior of Metal-Oxide/2D-Material Contacts. Tribology Letters, 2021, 69, 1.	2.6	8
31	Importance of quadratic dispersion in acoustic flexural phonons for thermal transport of two-dimensional materials. Physical Review B, 2021, 103, .	3.2	38
32	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
33	Neural evolution structure generation: High entropy alloys. Journal of Chemical Physics, 2021, 155, 044102.	3.0	5
34	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
35	Two-Dimensional Graphdiyne-Confined Platinum Catalyst for Hydrogen Evolution and Oxygen Reduction Reactions. ACS Applied Materials & Interfaces, 2021, 13, 47541-47548.	8.0	15
36	Fatigue resistance of atomically thin graphene oxide. Carbon, 2021, 183, 780-788.	10.3	14

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37	Quantum well states and sizable Rashba splitting on Pb induced α-phase Bi/Si(111) surface reconstruction. Nanoscale, 2021, 13, 16622-16628.	5.6	5
38	Friction of magnetene, a non–van der Waals 2D material. Science Advances, 2021, 7, eabk2041.	10.3	21
39	Eggshell-like MoS ₂ Nanostructures with Negative Curvature and Stepped Faces for Efficient Hydrogen Evolution Reactions. ACS Applied Nano Materials, 2021, 4, 14086-14093.	5.0	5
40	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
41	Performance Analysis of Composite Helicopter Blade Using Synergistic Damage Mechanics Approach. AIAA Journal, 2020, 58, 968-976.	2.6	7
42	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
43	Temperature dependence of grain boundary excess free volume. Scripta Materialia, 2020, 178, 71-76.	5.2	29
44	Strength of graphene with curvilinear grain boundaries. Carbon, 2020, 158, 808-817.	10.3	11
45	Neural Network-Assisted Development of High-Entropy Alloy Catalysts: Decoupling Ligand and Coordination Effects. Matter, 2020, 3, 1318-1333.	10.0	83
46	Electrolyte-Phobic Surface for the Next-Generation Nanostructured Battery Electrodes. Nano Letters, 2020, 20, 7455-7462.	9.1	25
47	Transition metal–N ₄ embedded black phosphorus carbide as a high-performance bifunctional electrocatalyst for ORR/OER. Nanoscale, 2020, 12, 18721-18732.	5.6	39
48	Phase Evolution of a Prenucleator for Fast Li Nucleation in Allâ€Solidâ€State Lithium Batteries. Advanced Energy Materials, 2020, 10, 2001191.	19.5	17
49	Computational screening of homo and hetero transition metal dimer catalysts for reduction of CO ₂ to C ₂ products with high activity and low limiting potential. Journal of Materials Chemistry A, 2020, 8, 21241-21254.	10.3	51
50	Materials perspective on new lithium chlorides and bromides: insights into thermo-physical properties. Physical Chemistry Chemical Physics, 2020, 22, 22758-22767.	2.8	15
51	Structureâ€Dependent Wear and Shear Mechanics of Nanostructured MoS ₂ Coatings. Advanced Materials Interfaces, 2020, 7, 1901870.	3.7	13
52	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
53	Determining the limiting factor of the electrochemical stability window for PEO-based solid polymer electrolytes: main chain or terminal –OH group?. Energy and Environmental Science, 2020, 13, 1318-1325.	30.8	342
54	A triple atom catalyst with ultrahigh loading potential for nitrogen electrochemical reduction. Journal of Materials Chemistry A, 2020, 8, 15086-15093.	10.3	48

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55	Effect of He on the Order-Disorder Transition in Ni3Al under Irradiation. Physical Review Letters, 2020, 124, 075901.	7.8	9
56	Fatigue of graphene. Nature Materials, 2020, 19, 405-411.	27.5	110
57	Dramatic improvement in the performance of graphene as Li/Na battery anodes with suitable electrolytic solvents. Carbon, 2020, 161, 570-576.	10.3	12
58	Toughening of graphene-based polymer nanocomposites via tuning chemical functionalization. Composites Science and Technology, 2020, 194, 108140.	7.8	44
59	Compression-induced resistance of singlet oxygen dissociation on phosphorene. Physical Review Materials, 2020, 4, .	2.4	0
60	Hindered surface diffusion of bonded molecular clusters mediated by surface defects. Physical Review Materials, 2020, 4, .	2.4	1
61	Atomic structure of Ni-Nb-Y amorphous alloys and water-surface adsorption characteristics. Computational Materials Science, 2019, 169, 109095.	3.0	3
62	Understanding the Independent and Interdependent Role of Water and Oxidation on the Tribology of Ultrathin Molybdenum Disulfide (MoS ₂). Advanced Materials Interfaces, 2019, 6, 1901246.	3.7	26
63	Kinetics of annealing-induced detwinning in chemical vapor deposited nickel. Acta Materialia, 2019, 178, 263-274.	7.9	9
64	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
65	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
66	Analysis of the Material Behavior of 3D Printed Laminates Via FFF. Experimental Mechanics, 2019, 59, 871-881.	2.0	45
67	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
68	Short-range structural origins of serration events in metallic glasses. Journal of Alloys and Compounds, 2019, 787, 840-850.	5.5	6
69	How Silver Grows on the Silicon (001) Surface: A Theoretical and Experimental Investigation. ACS Applied Electronic Materials, 2019, 1, 122-131.	4.3	4
70	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
71	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
72	Catalytic CO2 reduction by palladium-decorated silicon–hydride nanosheets. Nature Catalysis, 2019, 2, 46-54.	34.4	116

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73	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
74	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
75	Uncertainty analysis and estimation of robust AIREBO parameters for graphene. Carbon, 2019, 142, 300-310.	10.3	43
76	Phosphorene as a Catalyst for Highly Efficient Nonaqueous Li–Air Batteries. ACS Applied Materials & Interfaces, 2019, 11, 499-510.	8.0	27
77	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
78	Development of constitutive material model of 3D printed structure via FDM. Materials Today Communications, 2018, 15, 143-152.	1.9	94
79	Nonlinear fracture toughness measurement and crack propagation resistance of functionalized graphene multilayers. Science Advances, 2018, 4, eaao7202.	10.3	72
80	Ultrahigh Storage and Fast Diffusion of Na and K in Blue Phosphorene Anodes. ACS Applied Materials & Interfaces, 2018, 10, 8630-8639.	8.0	143
81	Borophene hydride: a stiff 2D material with high thermal conductivity and attractive optical and electronic properties. Nanoscale, 2018, 10, 3759-3768.	5.6	109
82	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
83	Twoâ€dimensional boron as an impressive lithiumâ€sulphur battery cathode material. Energy Storage Materials, 2018, 13, 80-87.	18.0	38
84	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
85	Highly Efficient Ambient Temperature CO ₂ Photomethanation Catalyzed by Nanostructured RuO ₂ on Silicon Photonic Crystal Support. Advanced Energy Materials, 2018, 8, 1702277.	19.5	58
86	Solar Fuels: Highly Efficient Ambient Temperature CO ₂ Photomethanation Catalyzed by Nanostructured RuO ₂ on Silicon Photonic Crystal Support (Adv. Energy Mater. 9/2018). Advanced Energy Materials, 2018, 8, 1870041.	19.5	7
87	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
88	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
89	Tailoring Surface Frustrated Lewis Pairs of In ₂ O _{3â^'} <i>_x</i> (OH) _y for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO ₂ by Isomorphous Substitution of In ³⁺ with Bi ³⁺ . Advanced Science, 2018, 5, 1700732.	11.2	91
90	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

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91	Assessing progressive failure in long wind turbine blades under quasi-static and cyclic loads. Renewable Energy, 2018, 119, 754-766.	8.9	29
92	Adsorption and diffusion of lithium polysulfides over blue phosphorene for Li–S batteries. Nanoscale, 2018, 10, 21335-21352.	5.6	69
93	Enhanced photothermal reduction of gaseous CO ₂ over silicon photonic crystal supported ruthenium at ambient temperature. Energy and Environmental Science, 2018, 11, 3443-3451.	30.8	83
94	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
95	Time-dependent damage analysis for viscoelastic-viscoplastic structural laminates under biaxial loading. Composite Structures, 2018, 203, 60-70.	5.8	5
96	Solar Fuels: Tailoring Surface Frustrated Lewis Pairs of In ₂ O _{3â^'} <i>_x</i> (OH) _y for Gasâ€Phase Heterogeneous Photocatalytic Reduction of CO ₂ by Isomorphous Substitution of In ³⁺ with Bi ³⁺ (Adv. Sci. 6/2018). Advanced Science, 2018, 5, 1870034.	11.2	3
97	2.7 Micromechanics of Damage Evolution in Laminates. , 2018, , 118-147.		Ο
98	First Principles Investigation of HCl, H ₂ , and Chlorosilane Adsorption on Cu ₃ Si Surfaces with Applications for Polysilicon Production. Journal of Physical Chemistry C, 2018, 122, 20252-20260.	3.1	9
99	Hydrogen storage in Li, Na and Ca decorated and defective borophene: a first principles study. RSC Advances, 2018, 8, 20748-20757.	3.6	64
100	The ideal strength of two-dimensional stanene may reach or exceed the Griffith strength estimate. Nanoscale, 2017, 9, 7055-7062.	5.6	29
101	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
102	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
103	A fast mollified impulse method for biomolecular atomistic simulations. Journal of Computational Physics, 2017, 333, 180-198.	3.8	0
104	Atomistic Origins of Ductility Enhancement in Metal Oxide Coated Silicon Nanowires for Liâ€lon Battery Anodes. Advanced Materials Interfaces, 2017, 4, 1700920.	3.7	23
105	Effect of matrix cracks and delamination on extension-twist coupling of thin pretwisted composite strips. Composite Structures, 2017, 180, 234-250.	5.8	4
106	Role of graphene in enhancing the mechanical properties of TiO ₂ /graphene heterostructures. Nanoscale, 2017, 9, 11678-11684.	5.6	22
107	Adsorption of Metallic, Metalloidic, and Nonmetallic Adatoms on Two-Dimensional C ₃ N. Journal of Physical Chemistry C, 2017, 121, 18575-18583.	3.1	111
108	A first principles study of hydrogen storage inÂlithium decorated defective phosphorene. International Journal of Hydrogen Energy, 2017, 42, 23018-23027.	7.1	56

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109	Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO ₂ with High Activity and Tailored Selectivity. Advanced Science, 2017, 4, 1700252.	11.2	97
110	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
111	Photothermal Catalysis: Photothermal Catalyst Engineering: Hydrogenation of Gaseous CO ₂ with High Activity and Tailored Selectivity (Adv. Sci. 10/2017). Advanced Science, 2017, 4, .	11.2	2
112	Phosphorene as a Polysulfide Immobilizer and Catalyst in Highâ€Performance Lithium–Sulfur Batteries. Advanced Materials, 2017, 29, 1602734.	21.0	289
113	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
114	Self-Trapped Charge Carriers in Defected Amorphous TiO ₂ . Journal of Physical Chemistry C, 2016, 120, 27910-27916.	3.1	17
115	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
116	Vertically Oriented Arrays of ReS ₂ Nanosheets for Electrochemical Energy Storage and Electrocatalysis. Nano Letters, 2016, 16, 3780-3787.	9.1	241
117	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
118	Mechanical properties of monolayer penta-graphene and phagraphene: a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 26736-26742.	2.8	106
119	New insights into the structure-nonlinear mechanical property relations for graphene allotropes. Carbon, 2016, 110, 443-457.	10.3	32
120	Surface Analogues of Molecular Frustrated Lewis Pairs in Heterogeneous CO ₂ Hydrogenation Catalysis. ACS Catalysis, 2016, 6, 5764-5770.	11.2	80
121	Metadynamics-Biased ab Initio Molecular Dynamics Study of Heterogeneous CO ₂ Reduction via Surface Frustrated Lewis Pairs. ACS Catalysis, 2016, 6, 7109-7117.	11.2	78
122	Heterogeneous reduction of carbon dioxide by hydride-terminated silicon nanocrystals. Nature Communications, 2016, 7, 12553.	12.8	93
123	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
124	Photoexcited Surface Frustrated Lewis Pairs for Heterogeneous Photocatalytic CO ₂ Reduction. Journal of the American Chemical Society, 2016, 138, 1206-1214.	13.7	210
125	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
126	Interfacial Shear Strength of Multilayer Graphene Oxide Films. ACS Nano, 2016, 10, 1939-1947.	14.6	64

8

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127	Competing twinning mechanisms in body-centered cubic metallic nanowires. Scripta Materialia, 2016, 113, 214-217.	5.2	37
128	Critical stiffness damage envelopes for multidirectional laminated structures under multiaxial loading conditions. Materials and Design, 2016, 91, 218-229.	7.0	13
129	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
130	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
131	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
132	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
133	Failure mechanisms in thin-walled nanocrystalline cylinders under uniaxial compression. Acta Materialia, 2015, 86, 157-168.	7.9	0
134	A synergistic damage mechanics based multiscale model for composite laminates subjected to multiaxial strains. Mechanics of Materials, 2015, 83, 72-89.	3.2	42
135	Predicting evolution of ply cracks in composite laminates subjected toÂbiaxial loading. Composites Part B: Engineering, 2015, 75, 264-273.	12.0	48
136	llluminating CO ₂ reduction on frustrated Lewis pair surfaces: investigating the role of surface hydroxides and oxygen vacancies on nanocrystalline In ₂ O _{3â[°]x} (OH) _y . Physical Chemistry Chemical Physics, 2015, 17, 14623-14635.	2.8	186
137	Adsorption and Dissociation of H ₂ O on Monolayered MoS ₂ Edges: Energetics and Mechanism from <i>ab Initio</i> Simulations. Journal of Physical Chemistry C, 2015, 119, 6518-6529.	3.1	107
138	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
139	A Foldable Lithium–Sulfur Battery. ACS Nano, 2015, 9, 11342-11350.	14.6	125
140	Strengthening in Graphene Oxide Nanosheets: Bridging the Gap between Interplanar and Intraplanar Fracture. Nano Letters, 2015, 15, 6528-6534.	9.1	61
141	Effects of topological point reconstructions on the fracture strength and deformation mechanisms of graphene. Computational Materials Science, 2015, 97, 172-180.	3.0	23
142	High strength measurement of monolayer graphene oxide. Carbon, 2015, 81, 497-504.	10.3	138
143	Development of a Synergistic Damage Mechanics-Based Model for Predicting Multiaxial Effects in Progressive Failure of Composite Structures. , 2014, , .		Ο
144	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

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145	A kinematic study of energy barriers for crack formation in graphene tilt boundaries. Journal of Applied Physics, 2014, 115, .	2.5	19
146	Defect engineering of graphene for effective hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 4981-4995.	7.1	96
147	Progressive Failure Analysis of Polymer Composites Using a Synergistic Damage Mechanics Methodology. , 2014, , 147-155.		2
148	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
149	A DFT + <i>U</i> study of (Rh, Nb)-codoped rutile TiO ₂ . Journal of Physics Condensed Matter, 2013, 25, 085501.	1.8	23
150	Effect of doping on electronic structure and photocatalytic behavior of amorphous TiO2. Journal of Physics Condensed Matter, 2013, 25, 475501.	1.8	30
151	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
152	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
153	Atomistic simulations of dislocation–precipitate interactions emphasize importance of cross-slip. Scripta Materialia, 2011, 64, 398-401.	5.2	58
154	Mechanisms of Guinier–Preston zone hardening in the athermal limit. Acta Materialia, 2010, 58, 5797-5805.	7.9	81
155	Evolution of ply cracks in multidirectional composite laminates. International Journal of Solids and Structures, 2010, 47, 1338-1349.	2.7	86
156	A synergistic damage mechanics approach for composite laminates with matrix cracks in multiple orientations. Mechanics of Materials, 2009, 41, 954-968.	3.2	85
157	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
158	Analysis of multiple off-axis ply cracks in composite laminates. International Journal of Solids and Structures, 2008, 45, 4574-4589.	2.7	61
159	Multiscale Modeling for Damage Analysis. , 2008, , 529-578.		4
160	Damage Mechanics of Composite Laminates with Transverse Matrix Cracks in Multiple Orientations. , 2007, , .		2
161	Macro-damage mechanics. , 0, , 134-178.		0
162	Damage progression. , 0, , 179-236.		0