Nabil Khossossi

List of Publications by Year
in descending order

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332	11,961	34105	42399
papers	citations	52 h-index	92 g-index

340	340	340	13760
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dimensionality effects in highâ€performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1547.	14.6	20
2	Exploring the relationship between Ln leaching and Lnâ€“O binding energy in monazite (Nd, Sm, Eu). Journal of the American Ceramic Society, 2022, 105, 553-563.	3.8	5
3	Preparation and properties of situ-sintered SiC ceramics aided by ZnO-Al2O3-CaO. Journal of Alloys and Compounds, 2022, 890, 161854.	5.5	1
4	Asymmetry-Induced Redistribution in Sn(IV)â€“Ti(IV) Hetero-Bimetallic Alkoxide Precursors and Its Impact on Thin-Film Deposition by Metalâ€“Organic Chemical Vapor Deposition. Crystal Growth and Design, 2022, 22, 54-59.	3.0	1
5	Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis. Green Chemistry, 2022, 24, 1190-1210.	9.0	23
6	Binding and optical characteristics of polycyclic aromatic hydrocarbons and their nitroderivatives adsorbed on the C₃N monolayer. New Journal of Chemistry, 2022, 46, 2245-2258.	2.8	7
7	Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. Journal of Materials Chemistry A, 2022, 10, 1569-1578.	10.3	13
8	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solidâ€“liquid interfaces. Nanoscale Advances, 2022, 4, 884-893.	4.6	4
9	Two-Dimensional Perovskite/HfS₂ van der Waals Heterostructure as an Absorber Material for Photovoltaic Applications. ACS Applied Energy Materials, 2022, 5, 2300-2307.	5.1	9
10	Modified KBBF-like Material for Energy Storage Applications: ZnNiBO₃(OH) with Enhanced Cycle Life. ACS Applied Materials & Interfaces, 2022, 14, 8025-8035.	8.0	20
11	Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer $$WS_2$$. Scientific Reports, 2022, 12, 2593.	3.3	10
12	Relativistic Effects in Platinum Nanocluster Catalysis: A Statistical Ensemble-Based Analysis. Journal of Physical Chemistry A, 2022, 126, 1345-1359.	2.5	7
13	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. ACS Applied Nano Materials, 2022, 5, 2984-2993.	5.0	29
14	Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ2 (Qâ€‰=â€‰S, Se) monolayer. Scientific Reports, 2022, 12, 2964.	3.3	19
15	Dynamical modeling of miR-34a, miR-449a, and miR-16 reveals numerous DDR signaling pathways regulating senescence, autophagy, and apoptosis in HeLa cells. Scientific Reports, 2022, 12, 4911.	3.3	15
16	Preparation and dielectric properties of La doped NBCCTO ceramics. Journal of Electroceramics, 2022, 48, 117-126.	2.0	4
17	Progress and challenges in layered two-dimensional hybrid perovskites. Nanotechnology, 2022, 33, 292501.	2.6	11
18	Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries. Nano Energy, 2022, 96, 107066.	16.0	29

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19	2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications. Materials Today Advances, 2022, 14, 100225.	5.2	10
20	Janus Aluminum Oxysulfide Al2OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. Applied Surface Science, 2022, 589, 152997.	6.1	21
21	Antibodies Against Phosphorylcholine Among 60-Year-Olds: Clinical Role and Simulated Interactions. Frontiers in Cardiovascular Medicine, 2022, 9, 809007.	2.4	6
22	Stabilizing superconductivity of ternary metal pentahydride $$hbox {CaCH}_{{5}}$$ via electronic topological transitions under high pressure from first principles evolutionary algorithm. Scientific Reports, 2022, 12, 6700.	3.3	3
23	Activationâ€Induced Surface Modulation of Biowasteâ€Derived Hierarchical Porous Carbon for Supercapacitors. ChemPlusChem, 2022, 87, .	2.8	18
24	Bifunctional catalytic activity of 2D boron monochalcogenides BX (XÂ=ÂS, Se, Te). Materials Today Energy, 2022, 27, 101026.	4.7	7
25	Prominent Electrode Material for Na-, K-, and Mg-ion Batteries: 2D Î²-Sb Monolayer. Energy & Fuels, 2022, 36, 7087-7095.	5.1	16
26	Tuning the electronic, magnetic, and sensing properties of a single atom embedded microporous C₃N₆ monolayer towards XO₂ (X = C, N, S) gases. New Journal of Chemistry, 2022, 46, 13752-13765.	2.8	5
27	Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER catalyst under external electric field influence. Catalysis Today, 2021, 370, 14-25.	4.4	20
28	Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX2 monolayer. Journal of Materials Science, 2021, 56, 3846-3860.	3.7	24
29	Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure. Physica Status Solidi (B): Basic Research, 2021, 258, 2000279.	1.5	8
30	Mechanism of formaldehyde and formic acid formation on (101)-TiO₂@Cu₄ systems through CO₂ hydrogenation. Sustainable Energy and Fuels, 2021, 5, 564-574.	4.9	4
31	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
32	Cs2InGaX6 (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics. Current Applied Physics, 2021, 21, 50-57.	2.4	48
33	No-Carbon 2D Anode Materials for Next-Generation Batteries. , 2021, , 1-14.		0
34	Hydrogenation and oxidation enhances the thermoelectric performance of Si₂BN monolayer. New Journal of Chemistry, 2021, 45, 3892-3900.	2.8	8
35	Pressure-promoted highly-ordered Fe-doped-Ni₂B for effective oxygen evolution reaction and overall water splitting. Journal of Materials Chemistry A, 2021, 9, 6469-6475.	10.3	37
36	Data-Driven Machine Learning Approaches for Advanced Battery Modeling. , 2021, , 1-18.		0

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37	Determining factors for the nano-biocompatibility of cobalt oxide nanoparticles: proximal discrepancy in intrinsic atomic interactions at differential vicinage. Green Chemistry, 2021, 23, 3439-3458.	9.0	38
38	Formation of Lightweight Ternary Polyhydrides and Their Hydrogen Storage Mechanism. Journal of Physical Chemistry C, 2021, 125, 1723-1730.	3.1	19
39	MXene-Based 2D Anode Materials for Next-Generation Batteries. , 2021, , 1-20.		1
40	Design of Continuous Transport of the Droplet by the Contact-Boiling Regime. Langmuir, 2021, 37, 553-560.	3.5	8
41	Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO₂ Resistive Random Access Memory Device. Journal of Physical Chemistry Letters, 2021, 12, 1876-1884.	4.6	20
42	8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. Physical Review B, 2021, 103, .	3.2	26
43	Stabilization and electronic topological transition of hydrogen-rich metal Li5MoH11 under high pressures from first-principles predictions. Scientific Reports, 2021, 11, 4079.	3.3	12
44	Large-Scale Fabrication of Wettability-Controllable Coatings for Optimizing Condensate Transfer Ability. Langmuir, 2021, 37, 2476-2484.	3.5	4
45	Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. Nanomedicine, 2021, 16, 307-322.	3.3	9
46	Large-Scale Screening of Interface Parameters in the WC/W System Using Classical Force Field and First-Principles Calculations. Journal of Physical Chemistry C, 2021, 125, 3631-3639.	3.1	3
47	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. ACS Applied Electronic Materials, 2021, 3, 733-742.	4.3	13
48	Mechanistic Understanding of the Interactions and Pseudocapacitance of Multiâ€Electron Redox Organic Molecules Sandwiched between MXene Layers. Advanced Electronic Materials, 2021, 7, 2001202.	5.1	10
49	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. Energy & Fuels, 2021, 35, 6282-6288.	5.1	10
50	Salt-assisted growth of monolayer MoS2 for high-performance hysteresis-free field-effect transistor. Journal of Applied Physics, 2021, 129, .	2.5	19
51	Carbon Nitride Monolayers as Efficient Immobilizers toward Lithium Selenides: Potential Applications in Lithiumâ€“Selenium Batteries. ACS Applied Energy Materials, 2021, 4, 3891-3904.	5.1	10
52	Antimonene Allotropes Î±- and Î²-Phases as Promising Anchoring Materials for Lithiumâ€“Sulfur Batteries. Energy & Fuels, 2021, 35, 9001-9009.	5.1	15
53	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. International Journal of Hydrogen Energy, 2021, 46, 20586-20593.	7.1	17
54	Degradation of Alzheimerâ€™s Amyloid-Î² by a Catalytically Inactive Insulin-Degrading Enzyme. Journal of Molecular Biology, 2021, 433, 166993.	4.2	27

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55	Understanding carbon dioxide capture on metalâ€“organic frameworks from first-principles theory: The case of MIL-53(X), with X = Fe3+, Al3+, and Cu2+. Journal of Chemical Physics, 2021, 155, 024701.	3.0	6
56	Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. Journal of Computational Chemistry, 2021, 42, 1944-1958.	3.3	4
57	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. Applied Surface Science, 2021, 556, 149561.	6.1	31
58	High-Specific-Capacity and High-Performing Post-Lithium-Ion Battery Anode over 2D Black Arsenic Phosphorus. ACS Applied Energy Materials, 2021, 4, 7900-7910.	5.1	19
59	High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. Scientific Reports, 2021, 11, 16403.	3.3	9
60	Correlation between reduced dielectric loss and charge migration kinetics in NdFeO3-modified Ba0.7Sr0.3TiO3 ceramics. Journal of Materials Science: Materials in Electronics, 2021, 32, 24910.	2.2	2
61	Nitrogen-Containing Gas Sensing Properties of 2-D Ti2N and Its Derivative Nanosheets: Electronic Structures Insight. Nanomaterials, 2021, 11, 2459.	4.1	5
62	Electric Field-Modulated Charge Transfer in Geometrically Tailored MoX₂/WX₂ (X = S, Se) Heterostructures. Journal of Physical Chemistry C, 2021, 125, 22360-22369.	3.1	15
63	Coexisting commensurate and incommensurate charge ordered phases in CoO. Scientific Reports, 2021, 11, 19415.	3.3	0
64	Two-dimensional Janus Sn2SSe and SnGeS2 semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations. Physica E: Low-Dimensional Systems and Nanostructures, 2021, 134, 114900.	2.7	20
65	Influence of vacancy and adatom defects on the optoelectronic properties of monolayer GeS. AIP Conference Proceedings, 2021, , .	0.4	0
66	Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. Catalysis Science and Technology, 2021, 11, 4996-5013.	4.1	18
67	Metallic one-dimensional heterostructure for gas molecule sensing. Scientific Reports, 2021, 11, 433.	3.3	2
68	MXene binder stabilizes pseudocapacitance of conducting polymers. Journal of Materials Chemistry A, 2021, 9, 20356-20361.	10.3	15
69	Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. Journal of Materials Chemistry A, 2021, 9, 21291-21301.	10.3	18
70	Harnessing the unique properties of MXenes for advanced rechargeable batteries. JPhys Energy, 2021, 3, 012005.	5.3	14
71	Pressure-induced orderâ€“disorder transitions in Î²-In₂S₃: an experimental and theoretical study of structural and vibrational properties. Physical Chemistry Chemical Physics, 2021, 23, 23625-23642.	2.8	3
72	Polypeptoid Material as an Anchoring Material for Liâ€“S Batteries. ACS Applied Energy Materials, 2021, 4, 13070-13076.	5.1	8

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73	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space. ACS Omega, 2021, 6, 33240-33252.	3.5	9
74	Tuning the Nanoparticle Interfacial Properties and Stability of the Coreâ€“Shell Structure in Zn-Doped NiMoO₄@AWO₄. ACS Applied Materials & Interfaces, 2021, 13, 56116-56130.	8.0	30
75	Theoretical Prediction of a Bi-Doped Î²-Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. ACS Applied Materials & Interfaces, 2021, 13, 56254-56264.	8.0	10
76	Fabrication of BP2T functionalized graphene via non-covalent Ï€â€“Ï€ stacking interactions for enhanced ammonia detection. RSC Advances, 2021, 11, 35982-35987.	3.6	2
77	Progress in supercapacitors: roles of two dimensional nanotubular materials. Nanoscale Advances, 2020, 2, 70-108.	4.6	164
78	Li-decorated carbyne for hydrogen storage: charge induced polarization and van't Hoff hydrogen desorption temperature. Sustainable Energy and Fuels, 2020, 4, 691-699.	4.9	24
79	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C3N4) nanosheets under selected transition metal doping. International Journal of Hydrogen Energy, 2020, 45, 3035-3045.	7.1	110
80	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. Materials Today, 2020, 32, 108-130.	14.2	271
81	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. Catalysts, 2020, 10, 1111.	3.5	35
82	Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. Journal of Physical Chemistry C, 2020, 124, 22173-22184.	3.1	10
83	Tunning Hydrogen Storage Properties of Carbon Eneâ€“Yne Nanosheets through Selected Foreign Metal Functionalization. Journal of Physical Chemistry C, 2020, 124, 16827-16837.	3.1	15
84	Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density Liâ€“S Batteries. ACS Applied Energy Materials, 2020, 3, 7306-7317.	5.1	23
85	Coreâ€“shell nanostructures: perspectives towards drug delivery applications. Journal of Materials Chemistry B, 2020, 8, 8992-9027.	5.8	127
86	Emerging piezochromism in transparent lead free perovskite Rb3X2I9 (Xâ€‰=â€‰Sb, Bi) under compression: A comparative theoretical insight. Journal of Applied Physics, 2020, 128, 045102.	2.5	5
87	Ultrathin nanowire PdX₂ (X = P, As): stability, electronic transport and thermoelectric properties. New Journal of Chemistry, 2020, 44, 15617-15624.	2.8	3
88	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS₃ (A =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	5.5	24
89	Route to high-$$T_{c}$$ superconductivity of $$hbox {BC}_{{7}}$$ via strong bonding of boronâ€“carbon compound at high pressure. Scientific Reports, 2020, 10, 18090.	3.3	11
90	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. ChemCatChem, 2020, 12, 6013-6023.	3.7	20

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91	Temperature-Dependent Cationic Doping-Driven Phonon Dynamics Investigation in CdO Thin Films Using Raman Spectroscopy. Journal of Physical Chemistry C, 2020, 124, 21818-21828.	3.1	4
92	Toroidal Metaphotonics and Metadevices. Laser and Photonics Reviews, 2020, 14, 1900326.	8.7	95
93	Zn Metal Atom Doping on the Surface Plane of One-Dimesional NiMoO₄ Nanorods with Improved Redox Chemistry. ACS Applied Materials & Interfaces, 2020, 12, 44815-44829.	8.0	67
94	Optical excitations and thermoelectric properties of two-dimensional holey graphene. Physical Review B, 2020, 102, .	3.2	28
95	Recent progress of defect chemistry on 2D materials for advanced battery anodes. Chemistry - an Asian Journal, 2020, 15, 3390-3404.	3.3	35
96	Density Functional Theory Studies of Si₂BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. ACS Applied Nano Materials, 2020, 3, 9055-9063.	5.0	40
97	Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Two-Dimensional Thallium Selenide. ACS Applied Energy Materials, 2020, 3, 9315-9325.	5.1	24
98	Elucidating hydrogen storage properties of two-dimensional siligraphene (SiC₈) monolayers upon selected metal decoration. Sustainable Energy and Fuels, 2020, 4, 5578-5587.	4.9	22
99	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se) Tj ETQq1 1 0.784314 rgBT /Ove	8.0	130
100	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. Nanomaterials, 2020, 10, 2554.	4.1	17
101	Poisonous Vapor Adsorption on Pure and Modified Aluminum Nitride Nanosheet for Environmental Safety: A DFT Exploration. Sustainability, 2020, 12, 10097.	3.2	3
102	Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte. ACS Applied Energy Materials, 2020, 3, 12385-12399.	5.1	21
103	First-Principles Exploration of Hazardous Gas Molecule Adsorption on Pure and Modified Al60N60 Nanoclusters. Nanomaterials, 2020, 10, 2156.	4.1	2
104	Revealing the veil of the stability of monolayer boron sulfide upon air and humidity exposure. AIP Conference Proceedings, 2020, , .	0.4	0
105	Mechanical and electronic properties of van der Waals layered hcp PdH2. Scientific Reports, 2020, 10, 8037.	3.3	3
106	Molecules versus Nanoparticles: Identifying a Reactive Molecular Intermediate in the Synthesis of Ternary Coinage Metal Chalcogenides. Inorganic Chemistry, 2020, 59, 7727-7738.	4.0	10
107	Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. Journal of Applied Physics, 2020, 127, .	2.5	19
108	Structural Phase Transitions, Electronic Properties, and Hardness of RuB₄ under High Pressure in Comparison with FeB₄ and OsB₄. Journal of Physical Chemistry C, 2020, 124, 14804-14810.	3.1	20

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109	Hydrogen storage characteristics of Li and Na decorated 2D boron phosphide. Sustainable Energy and Fuels, 2020, 4, 4538-4546.	4.9	49
110	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. Science Advances, 2020, 6, eabb8097.	10.3	138
111	Exploring the Possibility of Î²â€Phase Arsenicâ€Phosphorus Polymorph Monolayer as Anode Materials for Sodiumâ€Ion Batteries. Advanced Theory and Simulations, 2020, 3, 2000023.	2.8	14
112	Effect of Cycling Ion and Solvent on the Redox Chemistry of Substituted Quinones and Solvent-Induced Breakdown of the Correlation between Redox Potential and Electron-Withdrawing Power of Substituents. Journal of Physical Chemistry C, 2020, 124, 13609-13617.	3.1	22
113	Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field. International Journal of Hydrogen Energy, 2020, 45, 12384-12393.	7.1	24
114	Strain-Engineered Metal-Free h-B₂O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. Journal of Physical Chemistry C, 2020, 124, 7884-7892.	3.1	27
115	Carbides-anti-perovskites Mn3(Sn, Zn)C: Potential candidates for an application in magnetic refrigeration. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114317.	2.7	7
116	2D monolayer boron sulfide as an efficient material for optical nanodevices. AIP Conference Proceedings, 2020, , .	0.4	2
117	Electronic and optical properties of a structural defect in 2D MgF2 monolayer. AIP Conference Proceedings, 2020, , .	0.4	4
118	Capacity enhancement of polylithiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. Physical Chemistry Chemical Physics, 2020, 22, 15675-15682.	2.8	18
119	Van der Waals induced molecular recognition of canonical DNA nucleobases on a 2D GaS monolayer. Physical Chemistry Chemical Physics, 2020, 22, 6706-6715.	2.8	5
120	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. Sustainable Energy and Fuels, 2020, 4, 2363-2369.	4.9	62
121	Rectifying behavior in twisted bilayer black phosphorus nanojunctions mediated through intrinsic anisotropy. Nanoscale Advances, 2020, 2, 1493-1501.	4.6	13
122	Room-temperature conversion of Cu_{2â^'x}Se to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO₂. Dalton Transactions, 2020, 49, 3580-3591.	3.3	13
123	Exploring two-dimensional M2NS2 (Mâ€¯=â€¯Ti, V) MXenes based gas sensors for air pollutants. Applied Materials Today, 2020, 19, 100574.	4.3	44
124	HfS2 and TiS2 Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. Catalysts, 2020, 10, 94.	3.5	10
125	Necklaceâ€like Nitrogenâ€Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. Advanced Functional Materials, 2020, 30, 1909725.	14.9	89
126	Superior sensitivity of metal functionalized boron carbide (BC3) monolayer towards carbonaceous pollutants. Applied Surface Science, 2020, 512, 145637.	6.1	15

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127	Crystallography of low Z material at ultrahigh pressure: Case study on solid hydrogen. Matter and Radiation at Extremes, 2020, 5, .	3.9	15
128	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. Nanoscale Advances, 2020, 2, 2410-2421.	4.6	23
129	Impact of edge structures on interfacial interactions and efficient visible-light photocatalytic activity of metalâ€“semiconductor hybrid 2D materials. Catalysis Science and Technology, 2020, 10, 3279-3289.	4.1	37
130	Sensing the polar molecules MH3 (M = N, P, or As) with a Janus NbTeSe monolayer. New Journal of Chemistry, 2020, 44, 7932-7940.	2.8	20
131	Carbon-phosphide monolayer with high carrier mobility and perceptibleIâ€“Vresponse for superior gas sensing. New Journal of Chemistry, 2020, 44, 3777-3785.	2.8	23
132	Interplay of charge density wave and multiband superconductivity in layered quasi-two-dimensional materials: The case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>2</mml:mn><mml:mi mathvariant="normal">H</mml:mi><mml:mtext>â^'</mml:mtext><mml:mi>Nb</mml:mi><mml:msub><mml:mrow><mml:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>2</mml:mn><mml:mi mathva	2.4	36
133	Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS₂. ACS Applied Energy Materials, 2019, 2, 6891-6903.	5.1	31
134	Probing the active sites of newly predicted stable Janus scandium dichalcogenides for photocatalytic water-splitting. Catalysis Science and Technology, 2019, 9, 4981-4989.	4.1	28
135	Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries. Journal of Physical Chemistry C, 2019, 123, 19340-19346.	3.1	18
136	Ab initio 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
137	Defect Thermodynamics in Nonstoichiometric Alluaudite-Based Polyanionic Materials for Na-Ion Batteries. ACS Applied Materials & Interfaces, 2019, 11, 32856-32868.	8.0	5
138	Interfacial aspect of ZnTe/In₂Te₃ heterostructures as an efficient catalyst for the hydrogen evolution reaction. Journal of Materials Chemistry A, 2019, 7, 27441-27449.	10.3	41
139	Investigation of the Factors That Dictate the Preferred Orientation of Lexitropsins in the Minor Groove of DNA. Journal of Medicinal Chemistry, 2019, 62, 10423-10440.	6.4	7
140	Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and BiI₃. Inorganic Chemistry, 2019, 58, 12040-12052.	4.0	45
141	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. Journal of Materials Chemistry C, 2019, 7, 12312-12320.	5.5	85
142	Ab Initio Screening of Doped Mg(AlH4)2 Systems for Conversion-Type Lithium Storage. Materials, 2019, 12, 2599.	2.9	5
143	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe₂ and) Tj ETQq1 1 0.784314 rgBT /Ov	7.8	101
144	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. Nanomaterials, 2019, 9, 1420.	4.1	4

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145	Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage. Nanoscale Advances, 2019, 1, 565-580.	4.6	49
146	Mapping the sodium intercalation mechanism, electrochemical properties and structural evolution in non-stoichiometric alluaudite Na_{2+2Î´}Fe_{2â^'Î´}(SO₄)₃ cathode materials. Journal of Materials Chemistry A, 2019, 7, 17446-17455.	10.3	11
147	Hybrid-Functional Study of Native Defects and W/Mo-Doped in Monoclinic-Bismuth Vanadate. Journal of Physical Chemistry C, 2019, 123, 14508-14516.	3.1	9
148	Li-Functionalized Carbon Nanotubes for Hydrogen Storage: Importance of Size Effects. ACS Applied Nano Materials, 2019, 2, 3021-3030.	5.0	33
149	Groundâ€"state structure of semiconducting and superconducting phases in xenon carbides at high pressure. Scientific Reports, 2019, 9, 2459.	3.3	19
150	Aero-gel based CeO₂ nanoparticles: synthesis, structural properties and detailed humidity sensing response. Journal of Materials Chemistry C, 2019, 7, 5477-5487.	5.5	62
151	Modelling high-performing batteries with Mxenes: The case of S-functionalized two-dimensional nitride Mxene electrode. Nano Energy, 2019, 58, 877-885.	16.0	100
152	The influence of edge structure on the optoelectronic properties of Si2BN quantum dot. Journal of Applied Physics, 2019, 126, .	2.5	17
153	Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. Scientific Reports, 2019, 9, 17300.	3.3	18
154	Emergence of Si₂BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. ACS Applied Energy Materials, 2019, 2, 8441-8448.	5.1	18
155	Ultrahigh-pressure isostructural electronic transitions in hydrogen. Nature, 2019, 573, 558-562.	27.8	78
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