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	Defect Engineered g-C₃N₄ for Efficient Visible Light Photocatalytic Hydrogen Production. Chemistry of Materials, 2015, 27, 4930-4933.	6.7	401
2	Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. Journal of Physical Chemistry C, 2014, 118, 26560-26568.	3.1	383
3	Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. Catalysis Science and Technology, 2017, 7, 545-559.	4.1	345
4	Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS₂/AlN(GaN) Heterostructures. Journal of Physical Chemistry C, 2014, 118, 17594-17599.	3.1	340
5	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. ChemSusChem, 2015, 8, 2789-2825.	6.8	302
6	Physisorption of nucleobases on graphene: Density-functional calculations. Physical Review B, 2007, 76, .	3.2	296
7	Single-layer MoS2 as an efficient photocatalyst. Catalysis Science and Technology, 2013, 3, 2214.	4.1	271
8	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. Materials Today, 2020, 32, 108-130.	14.2	271
9	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
10	Experimental and Theoretical Identification of a New High-PressureTiO2Polymorph. Physical Review Letters, 2001, 87, 275501.	7.8	175
11	Highly Sensitive and Selective Gas Detection Based on Silicene. Journal of Physical Chemistry C, 2015, 119, 16934-16940.	3.1	174
12	Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. Physical Review B, 2005, 71, .	3.2	173
13	Progress in supercapacitors: roles of two dimensional nanotubular materials. Nanoscale Advances, 2020, 2, 70-108.	4.6	164
14	Li+ ion conductivity and diffusion mechanism in Î±-Li3N and Î²-Li3N. Energy and Environmental Science, 2010, 3, 1524.	30.8	149
15	Toward the Realization of 2D Borophene Based Gas Sensor. Journal of Physical Chemistry C, 2017, 121, 26869-26876.	3.1	148
16	A possible mechanism for the emergence of an additional band gap due to a Tiâ€“Oâ€“C bond in the TiO₂â€“graphene hybrid system for enhanced photodegradation of methylene blue under visible light. RSC Advances, 2014, 4, 59890-59901.	3.6	143
17	Borophane as a Benchmate of Graphene: A Potential 2D Material for Anode of Li and Na-Ion Batteries. ACS Applied Materials & Interfaces, 2017, 9, 16148-16158.	8.0	142
18	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. Science Advances, 2020, 6, eabb8097.	10.3	138

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19	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (X = Se) Tj ETQq1 1 0.784314 rgBT /Ove	8.0	130
20	Coreâ€“shell nanostructures: perspectives towards drug delivery applications. Journal of Materials Chemistry B, 2020, 8, 8992-9027.	5.8	127
21	The curious case of two dimensional Si2BN: A high-capacity battery anode material. Nano Energy, 2017, 41, 251-260.	16.0	121
22	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
23	Room temperature ferromagnetism in pristine MgO thin films. Applied Physics Letters, 2010, 96, .	3.3	105
24	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe₂ and) Tj ETQq0 0 0 rgBT /Overlock 10	7.8	101
25	Relativity and the Lead-Acid Battery. Physical Review Letters, 2011, 106, 018301.	7.8	100
26	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
27	Na_{2.44}Mn_{1.79}(SO₄)₃: a new member of the alluaudite family of insertion compounds for sodium ion batteries. Journal of Materials Chemistry A, 2015, 3, 18564-18571.	10.3	99
28	Toroidal Metaphotonics and Metadevices. Laser and Photonics Reviews, 2020, 14, 1900326.	8.7	95
29	Necklaceâ€like Nitrogenâ€Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. Advanced Functional Materials, 2020, 30, 1909725.	14.9	89
30	Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. Applied Physics Letters, 2016, 109, .	3.3	86
31	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. Journal of Materials Chemistry C, 2019, 7, 12312-12320.	5.5	85
32	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. ACS Applied Materials & Interfaces, 2017, 9, 17977-17991.	8.0	82
33	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. Journal of Physical Chemistry C, 2016, 120, 25256-25262.	3.1	81
34	Ultrahigh-pressure isostructural electronic transitions in hydrogen. Nature, 2019, 573, 558-562.	27.8	78
35	Ab initio calculations of the mechanical properties of Ti3SiC2. Applied Physics Letters, 2001, 79, 1450-1452.	3.3	73
36	Theoretical Confirmation of the High Pressure Simple Cubic Phase in Calcium. Physical Review Letters, 1995, 75, 3473-3476.	7.8	72

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37	Anion-Doped NaTaO₃ for Visible Light Photocatalysis. Journal of Physical Chemistry C, 2013, 117, 22518-22524.	3.1	71
38	Sensing Characteristics of Phosphorene Monolayers toward PH₃ and AsH₃ Gases upon the Introduction of Vacancy Defects. Journal of Physical Chemistry C, 2016, 120, 20428-20436.	3.1	71
39	2D-HfS₂as an efficient photocatalyst for water splitting. Catalysis Science and Technology, 2016, 6, 6605-6614.	4.1	71
40	Enhanced DNA Sequencing Performance Through Edgeâ€Hydrogenation of Graphene Electrodes. Advanced Functional Materials, 2011, 21, 2674-2679.	14.9	70
41	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
42	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
43	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
44	Ionothermal Synthesis of High-Voltage Alluaudite Na_{2+2x}Fe_{2-x}(SO₄)₃ Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. ACS Applied Materials & Interfaces, 2016, 8, 6982-6991.	8.0	66
45	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. Applied Physics Letters, 2018, 112, .	3.3	66
46	Non-transition-metal doped diluted magnetic semiconductors. Applied Physics Letters, 2009, 94, .	3.3	64
47	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
48	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. Sustainable Energy and Fuels, 2020, 4, 2363-2369.	4.9	62
49	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
50	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
51	Tunable Assembly of sp³ Crossâ€Linked 3D Graphene Monoliths: A Firstâ€Principles Prediction. Advanced Functional Materials, 2013, 23, 5846-5853.	14.9	59
52	Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. Applied Physics Letters, 2012, 101, .	3.3	55
53	Melting and liquid structure of aluminum oxide using a molecular-dynamics simulation. Physical Review E, 1998, 57, 1673-1676.	2.1	54
54	Reduction of shock-wave data with mean-field potential approach. Journal of Applied Physics, 2002, 92, 6616-6620.	2.5	53

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55	Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. ACS Sensors, 2018, 3, 867-874.	7.8	53
56	Na_{2.32}Co_{1.84}(SO₄)₃ as a new member of the alluaudite family of high-voltage sodium battery cathodes. Dalton Transactions, 2017, 46, 55-63.	3.3	52
57	A comparative study of hydrogen evolution reaction on pseudo-monolayer WS₂ and PtS₂: insights based on the density functional theory. Catalysis Science and Technology, 2017, 7, 687-692.	4.1	51
58	Titanium metal at high pressure: Synchrotron experiments andab initiocalculations. Physical Review B, 2004, 69, .	3.2	50
59	Coupling in nanolaminated ternary carbides studied by theoretical means: The influence of electronic potential approximations. Physical Review B, 2006, 73, .	3.2	50
60	Synthesis, and crystal and electronic structure of sodium metal phosphate for use as a hybrid capacitor in non-aqueous electrolyte. Dalton Transactions, 2015, 44, 20108-20120.	3.3	50
61	High performance material for hydrogen storage: Graphenelike Si2BN solid. International Journal of Hydrogen Energy, 2017, 42, 22942-22952.	7.1	50
62	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
63	Hydrogen storage characteristics of Li and Na decorated 2D boron phosphide. Sustainable Energy and Fuels, 2020, 4, 4538-4546.	4.9	49
64	Metallized siligraphene nanosheets (SiC7) as high capacity hydrogen storage materials. Nano Research, 2018, 11, 3802-3813.	10.4	48
65	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
66	Layered Perovskite Sr2Ta2O7 for Visible Light Photocatalysis: A First Principles Study. Journal of Physical Chemistry C, 2013, 117, 5043-5050.	3.1	47
67	Ab initio calculation of elastic constants of SiO2 stishovite and Î±-quartz. Journal of Chemical Physics, 1999, 111, 2071-2074.	3.0	45
68	Theoretical assessment of feasibility to sequence DNA through interlayer electronic tunneling transport at aligned nanopores in bilayer graphene. Scientific Reports, 2015, 5, 17560.	3.3	45
69	Borophene's tryst with stability: exploring 2D hydrogen boride as an electrode for rechargeable batteries. Physical Chemistry Chemical Physics, 2018, 20, 22008-22016.	2.8	45
70	Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and BiI₃. Inorganic Chemistry, 2019, 58, 12040-12052.	4.0	45
71	High pressure structural phase transitions in IVâ€“VI semiconductors. Physica Status Solidi (B): Basic Research, 2003, 235, 341-347.	1.5	44
72	Stability of the MgCO3 structures under lower mantle conditions. American Mineralogist, 2005, 90, 1008-1011.	1.9	44

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73	Substitution induced band structure shape tuning in hybrid perovskites (CH₃NH₃Pb_{1â^'x}Sn_xI₃) for efficient solar cell applications. RSC Advances, 2015, 5, 107497-107502.	3.6	44
74	Exploring two-dimensional M2NS2 (Mâ€¯=â€¯Ti, V) MXenes based gas sensors for air pollutants. Applied Materials Today, 2020, 19, 100574.	4.3	44
75	Cumulene molecular wire conductance from first principles. Physical Review B, 2010, 81, .	3.2	43
76	Prospects of Grapheneâ€“hBN Heterostructure Nanogap for DNA Sequencing. ACS Applied Materials & Interfaces, 2017, 9, 39945-39952.	8.0	42
77	Origin of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>p</mml:mi></mml:mrow></mml:math>-type conductivity in layered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>n</mml:mi></mml:mrow></mml:math>GeTe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>A</mml:mo><mml:mi>m</mml:mi></mml:mrow></mml:math>Sb<mml:math	3.2	41
78	Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing. Applied Physics Letters, 2012, 100, 023701.	3.3	41
79	Hexagonal Boron Nitride (hâ€BN) Sheets Decorated with OLi, ONa, and Li₂F Molecules for Enhanced Energy Storage. ChemPhysChem, 2017, 18, 513-518.	2.1	41
80	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
81	Theoretical prediction of a phase transition in gold. Physical Review B, 2001, 63, .	3.2	40
82	Optical gap and native point defects in kaolinite studied by the GGA-PBE, HSE functional, and GW approaches. Physical Review B, 2011, 84, .	3.2	40
83	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
84	Calculating carbon nanotubeâ€“catalyst adhesion strengths. Physical Review B, 2007, 75, .	3.2	39
85	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
86	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
87	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
88	Fast crystallization of chalcogenide glass for rewritable memories. Applied Physics Letters, 2008, 93, .	3.3	36
89	Establishing the most favorable metalâ€“carbon bond strength for carbon nanotube catalysts. Journal of Materials Chemistry C, 2015, 3, 3422-3427.	5.5	36
90	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

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91	Anomalous fcc Crystal Structure of Thorium Metal. Physical Review Letters, 1995, 75, 280-283.	7.8	35
92	Calculated high pressure crystal structure transformations for phosphorus. Physica Status Solidi (B): Basic Research, 2003, 235, 282-287.	1.5	35
93	Effective masses and electronic structure of diamond including electron correlation effects in first principles calculations using the GW-approximation. AIP Advances, 2011, 1, .	1.3	35
94	Pressure-induced topological insulating behavior in the ternary chalcogenide Ge<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Sb<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Te<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	3.2	35
95	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. Catalysts, 2020, 10, 1111.	3.5	35
96	Recent progress of defect chemistry on 2D materials for advanced battery anodes. Chemistry - an Asian Journal, 2020, 15, 3390-3404.	3.3	35
97	Stable nitride complex and molecular nitrogen in N doped amorphous Ge2Sb2Te5. Applied Physics Letters, 2008, 93, .	3.3	34
98	Li-Functionalized Carbon Nanotubes for Hydrogen Storage: Importance of Size Effects. ACS Applied Nano Materials, 2019, 2, 3021-3030.	5.0	33
99	Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer. ACS Applied Energy Materials, 2018, 1, 3571-3576.	5.1	32
100	High-pressure phase transformations in carbonates. Physical Review B, 2010, 82, .	3.2	31
101	Cerium; Crystal Structure and Position in The Periodic Table. Scientific Reports, 2014, 4, 6398.	3.3	31
102	Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS₂. ACS Applied Energy Materials, 2019, 2, 6891-6903.	5.1	31
103	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. Applied Surface Science, 2021, 556, 149561.	6.1	31
104	Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional Si₂BN. Physical Chemistry Chemical Physics, 2018, 20, 21716-21723.	2.8	30
105	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
106	High Pressure Theoretical Studies of Actinide Dioxides. High Pressure Research, 2002, 22, 471-474.	1.2	29
107	Enabling the Electrochemical Activity in Sodium Iron Metaphosphate [NaFe(PO₃)₃] Sodium Battery Insertion Material: Structural and Electrochemical Insights. Inorganic Chemistry, 2017, 56, 5918-5929.	4.0	29
108	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. ACS Applied Nano Materials, 2022, 5, 2984-2993.	5.0	29

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109	Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries. Nano Energy, 2022, 96, 107066.	16.0	29
110	Anisotropy in the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>V</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>GeC</mml:m by soft x-ray emission spectroscopy and first-principles theory. Physical Review B, 2008, 78, .	3.2	28
111	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
112	Optical excitations and thermoelectric properties of two-dimensional holey graphene. Physical Review B, 2020, 102, .	3.2	28
113	Ab initiostudy of the Cr2AlC(0001) surface. Applied Physics Letters, 2006, 88, 161913.	3.3	27
114	One-dimensional polymeric carbon structure based on five-membered rings in alkaline earth metal dicarbides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BeC</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>MgC</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:ms Physical Review B, 2010, 82, .	3.2	27
115	Understanding from First-Principles Why LiNH2BH3Â·NH3BH3 Shows Improved Dehydrogenation over LiNH2BH3 and NH3BH3. Journal of Physical Chemistry C, 2010, 114, 19089-19095.	3.1	27
116	Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO₄ photoanode by Wâ€“Ti codoping. Journal of Materials Chemistry A, 2018, 6, 16965-16974.	10.3	27
117	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
118	Degradation of Alzheimerâ€™s Amyloid-Î² by a Catalytically Inactive Insulin-Degrading Enzyme. Journal of Molecular Biology, 2021, 433, 166993.	4.2	27
119	Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia: First-principles calculations. Physical Review B, 2009, 80, .	3.2	26
120	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
121	Sensing Characteristics of a Grapheneâ€like Boron Carbide Monolayer towards Selected Toxic Gases. ChemPhysChem, 2015, 16, 3511-3517.	2.1	25
122	Density Functional Theory Study of Hydrogen Adsorption in a Tiâ€Decorated Mgâ€Based Metalâ€“Organic Frameworkâ€74. ChemPhysChem, 2016, 17, 879-884.	2.1	25
123	TiS₂ Monolayer as an Emerging Ultrathin Bifunctional Catalyst: Influence of Defects and Functionalization. ChemPhysChem, 2019, 20, 608-617.	2.1	24
124	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
125	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS₃ (A =) Tj ETQq1 1 0.784314 rgBT /Ove	5.5	24
126	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

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127	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
128	Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX2 monolayer. Journal of Materials Science, 2021, 56, 3846-3860.	3.7	24
129	Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 17050-17053.	7.1	23
130	Stability of Ar(H ₂) ₂ to 358 GPa. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3596-3600.	7.1	23
131	The ideal commensurate value of Sc and the superconducting phase under high pressure. Journal of Applied Physics, 2018, 124, 225901.	2.5	23
132	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
133	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. Nanoscale Advances, 2020, 2, 2410-2421.	4.6	23
134	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
135	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
136	Thermodynamic analysis of hydrogen sorption reactions in Liâ€“Mgâ€“Nâ€“H systems. Applied Physics Letters, 2008, 92, 021907.	3.3	22
137	Superionicity in the hydrogen storage material<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Li</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Molecular dynamics simulations. Physical Review B, 2009, 79, .	3.2	22
138	Improvement in Hydrogen Desorption from Î²â€•and Î³â€MgH₂ upon Transitionâ€Metal Doping. ChemPhysChem, 2015, 16, 2557-2561.	2.1	22
139	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
140	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
141	The Origin of the Distorted Close-Packed Elemental Structure of Indium. Angewandte Chemie - International Edition, 1999, 38, 2017-2020.	13.8	21
142	Nano-fabrication of molecular electronic junctions by targeted modification of metal-molecule bonds. Scientific Reports, 2015, 5, 14431.	3.3	21
143	Probing the pseudo-1-D ion diffusion in lithium titanium niobate anode for Li-ion battery. Physical Chemistry Chemical Physics, 2016, 18, 22323-22330.	2.8	21
144	Structural prediction of host-guest structure in lithium at high pressure. Scientific Reports, 2018, 8, 5278.	3.3	21

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145	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
146	Janus Aluminum Oxysulfide Al2OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. Applied Surface Science, 2022, 589, 152997.	6.1	21
147	Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. ChemCatChem, 2020, 12, 6013-6023.	3.7	20
148	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
149	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
150	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
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