

Nabil Khossossi

List of Publications by Citations

Source: <https://exaly.com/author-pdf/4269848/nabil-khossossi-publications-by-citations.pdf>

Version: 2024-04-24

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

320
papers

8,082
citations

45
h-index

77
g-index

340
ext. papers

9,985
ext. citations

5.4
avg, IF

6.71
L-index

#	Paper	IF	Citations
320	Strain Engineering for Phosphorene: The Potential Application as a Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 26560-26568	3.8	314
319	Defect Engineered g-C3N4 for Efficient Visible Light Photocatalytic Hydrogen Production. <i>Chemistry of Materials</i> , 2015 , 27, 4930-4933	9.6	308
318	Physisorption of nucleobases on graphene: Density-functional calculations. <i>Physical Review B</i> , 2007 , 76,	3.3	274
317	Design of High-Efficiency Visible-Light Photocatalysts for Water Splitting: MoS2/AlN(GaN) Heterostructures. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 17594-17599	3.8	269
316	Review of two-dimensional materials for photocatalytic water splitting from a theoretical perspective. <i>Catalysis Science and Technology</i> , 2017 , 7, 545-559	5.5	251
315	Hydrogen Storage Materials for Mobile and Stationary Applications: Current State of the Art. <i>ChemSusChem</i> , 2015 , 8, 2789-825	8.3	236
314	Single-layer MoS2 as an efficient photocatalyst. <i>Catalysis Science and Technology</i> , 2013 , 3, 2214	5.5	236
313	Experimental and theoretical identification of a new high-pressure TiO2 polymorph. <i>Physical Review Letters</i> , 2001 , 87, 275501	7.4	156
312	Terahertz plasmonics: The rise of toroidal metadevices towards immunobiosensings. <i>Materials Today</i> , 2020 , 32, 108-130	21.8	148
311	Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-Free and Emergent Hybrid Perovskites. <i>ACS Energy Letters</i> , 2017 , 2, 837-845	20.1	142
310	Highly Sensitive and Selective Gas Detection Based on Silicene. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 16934-16940	3.8	131
309	A possible mechanism for the emergence of an additional band gap due to a TiO2 bond in the TiO2/graphene hybrid system for enhanced photodegradation of methylene blue under visible light. <i>RSC Advances</i> , 2014 , 4, 59890-59901	3.7	113
308	Li+ ion conductivity and diffusion mechanism in Li3N and Li3N. <i>Energy and Environmental Science</i> , 2010 , 3, 1524	35.4	112
307	Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. <i>Physical Review B</i> , 2005 , 71,	3.3	105
306	Borophane as a Benchmark of Graphene: A Potential 2D Material for Anode of Li and Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 16148-16158	9.5	101
305	Toward the Realization of 2D Borophene Based Gas Sensor. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 26869-26876	3.8	98
304	Room temperature ferromagnetism in pristine MgO thin films. <i>Applied Physics Letters</i> , 2010 , 96, 232505	3.4	98

303	Structure-based drug designing and immunoinformatics approach for SARS-CoV-2. <i>Science Advances</i> , 2020 , 6, eabb8097	14.3	97
302	Progress in supercapacitors: roles of two dimensional nanotubular materials. <i>Nanoscale Advances</i> , 2020 , 2, 70-108	5.1	91
301	Na _{2.44} Mn _{1.79} (SO ₄) ₃ : a new member of the alluaudite family of insertion compounds for sodium ion batteries. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 18564-18571	13	82
300	Relativity and the lead-acid battery. <i>Physical Review Letters</i> , 2011 , 106, 018301	7.4	80
299	Ab initio calculations of the mechanical properties of Ti ₃ SiC ₂ . <i>Applied Physics Letters</i> , 2001 , 79, 1450-1452	3.4	71
298	Two-dimensional boron: Lightest catalyst for hydrogen and oxygen evolution reaction. <i>Applied Physics Letters</i> , 2016 , 109, 053903	3.4	71
297	The curious case of two dimensional Si ₂ BN: A high-capacity battery anode material. <i>Nano Energy</i> , 2017 , 41, 251-260	17.1	68
296	Theoretical confirmation of the high pressure simple cubic phase in calcium. <i>Physical Review Letters</i> , 1995 , 75, 3473-3476	7.4	68
295	Defect and Substitution-Induced Silicene Sensor to Probe Toxic Gases. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 25256-25262	3.8	63
294	Anion-Doped NaTaO ₃ for Visible Light Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 22518-22524	3.8	63
293	Modelling high-performing batteries with Mxenes: The case of S-functionalized two-dimensional nitride Mxene electrode. <i>Nano Energy</i> , 2019 , 58, 877-885	17.1	62
292	Effect of Transition Metal Cations on Stability Enhancement for Molybdate-Based Hybrid Supercapacitor. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 17977-17991	9.5	61
291	Core-shell nanostructures: perspectives towards drug delivery applications. <i>Journal of Materials Chemistry B</i> , 2020 ,	7.3	61
290	Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes. <i>Advanced Functional Materials</i> , 2011 , 21, 2674-2679	15.6	60
289	Non-transition-metal doped diluted magnetic semiconductors. <i>Applied Physics Letters</i> , 2009 , 94, 102504	3.4	60
288	Rationalizing the Hydrogen and Oxygen Evolution Reaction Activity of Two-Dimensional Hydrogenated Silicene and Germanene. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 1536-44	9.5	56
287	Sensing Characteristics of Phosphorene Monolayers toward PH ₃ and AsH ₃ Gases upon the Introduction of Vacancy Defects. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 20428-20436	3.8	52
286	2D-HfS ₂ as an efficient photocatalyst for water splitting. <i>Catalysis Science and Technology</i> , 2016 , 6, 6605-6614	5.6	52

285	Ionothermal Synthesis of High-Voltage Alluaudite $\text{Na}_{2+2x}\text{Fe}_{2-x}(\text{SO}_4)_3$ Sodium Insertion Compound: Structural, Electronic, and Magnetic Insights. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 6982-91	9.5	52
284	Toroidal Metaphotonics and Metadevices. <i>Laser and Photonics Reviews</i> , 2020 , 14, 1900326	8.3	51
283	Strain induced lithium functionalized graphane as a high capacity hydrogen storage material. <i>Applied Physics Letters</i> , 2012 , 101, 103907	3.4	49
282	Tunable Assembly of sp^3 Cross-Linked 3D Graphene Monoliths: A First-Principles Prediction. <i>Advanced Functional Materials</i> , 2013 , 23, 5846-5853	15.6	49
281	Ultrahigh-pressure isostructural electronic transitions in hydrogen. <i>Nature</i> , 2019 , 573, 558-562	50.4	47
280	Necklace-like Nitrogen-Doped Tubular Carbon 3D Frameworks for Electrochemical Energy Storage. <i>Advanced Functional Materials</i> , 2020 , 30, 1909725	15.6	46
279	Titanium metal at high pressure: Synchrotron experiments and ab initio calculations. <i>Physical Review B</i> , 2004 , 69,	3.3	46
278	An emerging Janus MoSeTe material for potential applications in optoelectronic devices. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 12312-12320	7.1	45
277	Coupling in nanolaminated ternary carbides studied by theoretical means: The influence of electronic potential approximations. <i>Physical Review B</i> , 2006 , 73,	3.3	45
276	Melting and liquid structure of aluminum oxide using a molecular-dynamics simulation. <i>Physical Review E</i> , 1998 , 57, 1673-1676	2.4	45
275	Aero-gel based CeO_2 nanoparticles: synthesis, structural properties and detailed humidity sensing response. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 5477-5487	7.1	44
274	2D lateral heterostructures of group-III monochalcogenide: Potential photovoltaic applications. <i>Applied Physics Letters</i> , 2018 , 112, 143902	3.4	43
273	Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride ($\text{g-C}_3\text{N}_4$) nanosheets under selected transition metal doping. <i>International Journal of Hydrogen Energy</i> , 2020 , 45, 3035-3045	6.7	43
272	A comparative study of hydrogen evolution reaction on pseudo-monolayer WS_2 and PtS_2 : insights based on the density functional theory. <i>Catalysis Science and Technology</i> , 2017 , 7, 687-692	5.5	42
271	Elemental Substitution of Two-Dimensional Transition Metal Dichalcogenides (MoSe and MoTe): Implications for Enhanced Gas Sensing. <i>ACS Sensors</i> , 2019 , 4, 2646-2653	9.2	42
270	Reduction of shock-wave data with mean-field potential approach. <i>Journal of Applied Physics</i> , 2002 , 92, 6616-6620	2.5	42
269	Designing strategies to tune reduction potential of organic molecules for sustainable high capacity battery application. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 4430-4454	13	41
268	Layered Perovskite $\text{Sr}_2\text{Ta}_2\text{O}_7$ for Visible Light Photocatalysis: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5043-5050	3.8	41

267	Cumulene molecular wire conductance from first principles. <i>Physical Review B</i> , 2010 , 81,	3-3	41
266	Ab initio calculation of elastic constants of SiO ₂ stishovite and Quartz. <i>Journal of Chemical Physics</i> , 1999 , 111, 2071-2074	3-9	40
265	NaCo(SO) as a new member of the alluaudite family of high-voltage sodium battery cathodes. <i>Dalton Transactions</i> , 2016 , 46, 55-63	4-3	39
264	Calculating carbon nanotube catalyst adhesion strengths. <i>Physical Review B</i> , 2007 , 75,	3-3	39
263	High pressure structural phase transitions in IV-VI semiconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2003 , 235, 341-347	1-3	39
262	Synthesis, and crystal and electronic structure of sodium metal phosphate for use as a hybrid capacitor in non-aqueous electrolyte. <i>Dalton Transactions</i> , 2015 , 44, 20108-20	4-3	38
261	Two-dimensional boron monochalcogenide monolayer for thermoelectric material. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 2363-2369	5-8	37
260	Metallized siligraphene nanosheets (SiC ₇) as high capacity hydrogen storage materials. <i>Nano Research</i> , 2018 , 11, 3802-3813	10	37
259	Substitution induced band structure shape tuning in hybrid perovskites (CH ₃ NH ₃ Pb _{1-x} Sn _x I ₃) for efficient solar cell applications. <i>RSC Advances</i> , 2015 , 5, 107497-107502	3-7	37
258	Theoretical assessment of feasibility to sequence DNA through interlayer electronic tunneling transport at aligned nanopores in bilayer graphene. <i>Scientific Reports</i> , 2015 , 5, 17560	4-9	35
257	Pressure-induced topological insulating behavior in the ternary chalcogenide Ge ₂ Sb ₂ Te ₅ . <i>Physical Review B</i> , 2011 , 84,	3-3	35
256	High Thermoelectric Performance in Two-Dimensional Janus Monolayer Material WS-X (= Se and Te). <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 46212-46219	9-5	35
255	Fast crystallization of chalcogenide glass for rewritable memories. <i>Applied Physics Letters</i> , 2008 , 93, 061913	3-13	34
254	Calculated high pressure crystal structure transformations for phosphorus. <i>Physica Status Solidi (B): Basic Research</i> , 2003 , 235, 282-287	1-3	34
253	Defected and Functionalized Germanene-based Nanosensors under Sulfur Comprising Gas Exposure. <i>ACS Sensors</i> , 2018 , 3, 867-874	9-2	33
252	High performance material for hydrogen storage: Graphenelike Si ₂ BN solid. <i>International Journal of Hydrogen Energy</i> , 2017 , 42, 22942-22952	6-7	33
251	Origin of p-type conductivity in layered nGeTe/mSb ₂ Te ₃ chalcogenide semiconductors. <i>Physical Review B</i> , 2011 , 83,	3-3	33
250	Stability of the MgCO ₃ structures under lower mantle conditions. <i>American Mineralogist</i> , 2005 , 90, 1008-1011	1-11	33

249	Double-functionalized nanopore-embedded gold electrodes for rapid DNA sequencing. <i>Applied Physics Letters</i> , 2012 , 100, 023701	3-4	32
248	Stable nitride complex and molecular nitrogen in N doped amorphous Ge ₂ Sb ₂ Te ₅ . <i>Applied Physics Letters</i> , 2008 , 93, 241908	3-4	32
247	Borophene's tryst with stability: exploring 2D hydrogen boride as an electrode for rechargeable batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22008-22016	3.6	31
246	Theoretical prediction of a phase transition in gold. <i>Physical Review B</i> , 2001 , 63,	3-3	31
245	Anomalous fcc crystal structure of thorium metal. <i>Physical Review Letters</i> , 1995 , 75, 280-283	7-4	31
244	Hexagonal Boron Nitride (h-BN) Sheets Decorated with OLi, ONa, and Li F Molecules for Enhanced Energy Storage. <i>ChemPhysChem</i> , 2017 , 18, 513-518	3-2	30
243	Prospects of Graphene-hBN Heterostructure Nanogap for DNA Sequencing. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 39945-39952	9-5	29
242	Effective masses and electronic structure of diamond including electron correlation effects in first principles calculations using the GW-approximation. <i>AIP Advances</i> , 2011 , 1, 032139	1-5	28
241	Interfacial aspect of ZnTe/In ₂ Te ₃ heterostructures as an efficient catalyst for the hydrogen evolution reaction. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 27441-27449	13	27
240	Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer. <i>ACS Applied Energy Materials</i> , 2018 , 1, 3571-3576	6-1	26
239	Ab initio study of a 2D h-BAs monolayer: a promising anode material for alkali-metal ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18328-18337	3-6	26
238	One-dimensional polymeric carbon structure based on five-membered rings in alkaline earth metal dicarbides BeC ₂ and MgC ₂ . <i>Physical Review B</i> , 2010 , 82,	3-3	26
237	Understanding from First-Principles Why LiNH ₂ BH ₃ /NH ₃ BH ₃ Shows Improved Dehydrogenation over LiNH ₂ BH ₃ and NH ₃ BH ₃ . <i>Journal of Physical Chemistry C</i> , 2010 , 114, 19089-19095	3-8	26
236	Zn Metal Atom Doping on the Surface Plane of One-Dimensional NiMoO Nanorods with Improved Redox Chemistry. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 44815-44829	9-5	26
235	Optical gap and native point defects in kaolinite studied by the GGA-PBE, HSE functional, and GW approaches. <i>Physical Review B</i> , 2011 , 84,	3-3	25
234	Energetics of Al doping and intrinsic defects in monoclinic and cubic zirconia: First-principles calculations. <i>Physical Review B</i> , 2009 , 80,	3-3	25
233	Anisotropy in the electronic structure of V ₂ GeC investigated by soft x-ray emission spectroscopy and first-principles theory. <i>Physical Review B</i> , 2008 , 78,	3-3	25
232	Enabling the Electrochemical Activity in Sodium Iron Metaphosphate [NaFe(PO)] Sodium Battery Insertion Material: Structural and Electrochemical Insights. <i>Inorganic Chemistry</i> , 2017 , 56, 5918-5929	5-1	24

231	Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage. <i>Nanoscale Advances</i> , 2019 , 1, 565-580	5.1	24
230	Establishing the most favorable metal-carbon bond strength for carbon nanotube catalysts. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 3422-3427	7.1	24
229	Cerium; crystal structure and position in the periodic table. <i>Scientific Reports</i> , 2014 , 4, 6398	4.9	24
228	High Pressure Theoretical Studies of Actinide Dioxides. <i>High Pressure Research</i> , 2002 , 22, 471-474	1.6	24
227	Impact of edge structures on interfacial interactions and efficient visible-light photocatalytic activity of metal-semiconductor hybrid 2D materials. <i>Catalysis Science and Technology</i> , 2020 , 10, 3279-3289	5.5	24
226	Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio Variation of CsI and BiI ₃ . <i>Inorganic Chemistry</i> , 2019 , 58, 12040-12052	5.1	23
225	High-pressure phase transformations in carbonates. <i>Physical Review B</i> , 2010 , 82,	3.3	23
224	Simultaneous enhancement in charge separation and onset potential for water oxidation in a BiVO ₄ photoanode by W ^{VI} codoping. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 16965-16974	13	22
223	Thermodynamic analysis of hydrogen sorption reactions in Li-Mg-Ni systems. <i>Applied Physics Letters</i> , 2008 , 92, 021907	3.4	22
222	Ab initio study of the Cr ₂ AlC(0001) surface. <i>Applied Physics Letters</i> , 2006 , 88, 161913	3.4	22
221	Hydrogen storage characteristics of Li and Na decorated 2D boron phosphide. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 4538-4546	5.8	21
220	Thermodynamics and kinetics of 2D g-GeC monolayer as an anode materials for Li/Na-ion batteries. <i>Journal of Power Sources</i> , 2021 , 485, 229318	8.9	21
219	Exploring two-dimensional M ₂ NS ₂ (M = Ti, V) MXenes based gas sensors for air pollutants. <i>Applied Materials Today</i> , 2020 , 19, 100574	6.6	20
218	Probing the active sites of newly predicted stable Janus scandium dichalcogenides for photocatalytic water-splitting. <i>Catalysis Science and Technology</i> , 2019 , 9, 4981-4989	5.5	20
217	Revealing an unusual transparent phase of superhard iron tetraboride under high pressure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 17050-3	11.5	20
216	Superionicity in the hydrogen storage material Li ₂ NH: Molecular dynamics simulations. <i>Physical Review B</i> , 2009 , 79,	3.3	20
215	Sensing Characteristics of a Graphene-like Boron Carbide Monolayer towards Selected Toxic Gases. <i>ChemPhysChem</i> , 2015 , 16, 3511-7	3.2	19
214	The Origin of the Distorted Close-Packed Elemental Structure of Indium. <i>Angewandte Chemie - International Edition</i> , 1999 , 38, 2017-2020	16.4	19

213	Achieving ultrahigh carrier mobilities and opening the band gap in two-dimensional SiBN. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 21716-21723	3.6	18
212	Nano-fabrication of molecular electronic junctions by targeted modification of metal-molecule bonds. <i>Scientific Reports</i> , 2015 , 5, 14431	4.9	18
211	Recent Advancements and Future Prospects in Ultrathin 2D Semiconductor-Based Photocatalysts for Water Splitting. <i>Catalysts</i> , 2020 , 10, 1111	4	18
210	Structural prediction of host-guest structure in lithium at high pressure. <i>Scientific Reports</i> , 2018 , 8, 5278	4.9	17
209	Enhanced Optoelectronic and Thermoelectric Properties by Intrinsic Structural Defects in Monolayer HfS ₂ . <i>ACS Applied Energy Materials</i> , 2019 , 2, 6891-6903	6.1	17
208	Epitaxial graphene monolayer and bilayers on Ru(0001): Ab initio calculations. <i>Physical Review B</i> , 2010 , 82,	3.3	17
207	Structurally induced insulator-metal transition in solid oxygen: A quasiparticle investigation. <i>Physical Review B</i> , 2008 , 77,	3.3	17
206	Stability of Ar(H) to 358 GPa. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 3596-3600	11.5	16
205	Pressure-induced zigzag phosphorus chain and superconductivity in boron monophosphide. <i>Scientific Reports</i> , 2015 , 5, 8761	4.9	16
204	Li-Functionalized Carbon Nanotubes for Hydrogen Storage: Importance of Size Effects. <i>ACS Applied Nano Materials</i> , 2019 , 2, 3021-3030	5.6	15
203	Density Functional Theory Study of Hydrogen Adsorption in a Ti-Decorated Mg-Based Metal-Organic Framework-74. <i>ChemPhysChem</i> , 2016 , 17, 879-84	3.2	15
202	Theoretical Investigation of Metallic Nanolayers For Charge-Storage Applications. <i>ACS Applied Energy Materials</i> , 2018 , 1, 3428-3433	6.1	15
201	Mechanistic study of Na-ion diffusion and small polaron formation in K ⁺ inkite Na ₂ Fe(SO ₄) ₂ ·2H ₂ O based cathode materials. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 21726-21739	13	15
200	Improvement in hydrogen desorption from β and ϵ MgH ₂ upon transition-metal doping. <i>ChemPhysChem</i> , 2015 , 16, 2557-61	3.2	15
199	Interplay of charge density wave and multiband superconductivity in layered quasi-two-dimensional materials: The case of 2H _{1-x} NbS ₂ and 2H _{1-x} NbSe ₂ . <i>Physical Review Materials</i> , 2020 , 4,	3.2	15
198	Carbon-phosphide monolayer with high carrier mobility and perceptible I _V response for superior gas sensing. <i>New Journal of Chemistry</i> , 2020 , 44, 3777-3785	3.6	15
197	Recent progress of defect chemistry on 2D materials for advanced battery anodes. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 3390-3404	4.5	15
196	Sensing the polar molecules MH ₃ (M = N, P, or As) with a Janus NbTeSe monolayer. <i>New Journal of Chemistry</i> , 2020 , 44, 7932-7940	3.6	15

195	The ideal commensurate value of S_c and the superconducting phase under high pressure. <i>Journal of Applied Physics</i> , 2018 , 124, 225901	2.5	15
194	Probing the pseudo-1-D ion diffusion in lithium titanium niobate anode for Li-ion battery. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 22323-30	3.6	14
193	Towards a new class of heavy ion doped magnetic semiconductors for room temperature applications. <i>Scientific Reports</i> , 2015 , 5, 17053	4.9	14
192	Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations. <i>Scientific Reports</i> , 2015 , 5, 10301	4.9	14
191	Electronic density-of-states of amorphous vanadium pentoxide films: Electrochemical data and density functional theory calculations. <i>Journal of Applied Physics</i> , 2014 , 115, 183701	2.5	14
190	Role of correlation and relativistic effects in MAX phases. <i>Journal of Materials Science</i> , 2012 , 47, 7615-7620	4.9	14
189	Origin of ferromagnetism in molybdenum dioxide from ab initio calculations. <i>Physical Review B</i> , 2010 , 81,	3.3	14
188	On the structural and energetic properties of the hydrogen absorber $\text{Li}_2\text{Mg}(\text{NH})_2$. <i>Applied Physics Letters</i> , 2007 , 91, 091924	3.4	14
187	TiS Monolayer as an Emerging Ultrathin Bifunctional Catalyst: Influence of Defects and Functionalization. <i>ChemPhysChem</i> , 2019 , 20, 608-617	3.2	14
186	Ground-state structure of semiconducting and superconducting phases in xenon carbides at high pressure. <i>Scientific Reports</i> , 2019 , 9, 2459	4.9	13
185	Sensitive and selective detection of copper ions using low cost nitrogen doped carbon quantum dots as a fluorescent sensing platform. <i>ISSS Journal of Micro and Smart Systems</i> , 2017 , 6, 109-117	0.9	13
184	Cooperative Gold Nanoparticle Stabilization by Acetylenic Phosphaalkenes. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 10634-8	16.4	13
183	Formation and electronic properties of palladium hydrides and palladium-rhodium dihydride alloys under pressure. <i>Scientific Reports</i> , 2017 , 7, 3520	4.9	13
182	Hybrid density functional study of electronic and optical properties of phase change memory material: $\text{Ge}_2\text{Sb}_2\text{Te}_5$. <i>Journal of Applied Physics</i> , 2013 , 113, 033510	2.5	13
181	Differential conductance as a promising approach for rapid DNA sequencing with nanopore-embedded electrodes. <i>Applied Physics Letters</i> , 2010 , 97, 043701	3.4	13
180	$\text{Cs}_2\text{InGaX}_6$ (X=Cl, Br, or I): Emergent Inorganic Halide Double Perovskites with enhanced optoelectronic characteristics. <i>Current Applied Physics</i> , 2021 , 21, 50-57	2.6	13
179	Assessing the electrochemical properties of polypyridine and polythiophene for prospective applications in sustainable organic batteries. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3307-3314	3.6	12
178	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. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 13609-13617	3.8	12

- 177 Enhancement of hydrogen storage capacity on co-functionalized GaS monolayer under external electric field. *International Journal of Hydrogen Energy*, **2020**, 45, 12384-12393 6.7 12
- 176 Divulging the Hidden Capacity and Sodiation Kinetics of Na_xC₆Cl₄O₂: A High Voltage Organic Cathode for Sodium Rechargeable Batteries. *Journal of Physical Chemistry C*, **2017**, 121, 14027-14036 3.8 12
- 175 Polyfulvenes: Polymers with Handles That Enable Extensive Electronic Structure Tuning. *Journal of Physical Chemistry C*, **2015**, 119, 25726-25737 3.8 12
- 174 Energetics and magnetic properties of V-doped MgO bulk and (001) surface: A GGA, GGA+U, and hybrid density functional study. *Physical Review B*, **2010**, 82, 3.3 12
- 173 CRYSTALLOGRAPHIC STRUCTURES OF PbWO₄. *High Pressure Research*, **2003**, 23, 343-347 1.6 12
- 172 Electronic, elastic, and optical properties of Y₂O₂S. *Journal of Applied Physics*, **2005**, 97, 103711 2.5 12
- 171 Structural Insight of the Frailty of 2D Janus NbSeTe as an Active Photocatalyst. *ChemCatChem*, **2020**, 12, 6013-6023 5.2 12
- 170 Optical excitations and thermoelectric properties of two-dimensional holey graphene. *Physical Review B*, **2020**, 102, 3.3 12
- 169 Unveiling the thermodynamic and kinetic properties of Na_xFe(SO₄)₂ (x = 0.2): toward a high-capacity and low-cost cathode material. *Journal of Materials Chemistry A*, **2016**, 4, 17960-17969 13 12
- 168 Dynamic magneto-caloric effect of a multilayer nanographene: Dynamic quantum Monte Carlo. *Physica E: Low-Dimensional Systems and Nanostructures*, **2019**, 105, 139-145 3 12
- 167 Crystallography of low Z material at ultrahigh pressure: Case study on solid hydrogen. *Matter and Radiation at Extremes*, **2020**, 5, 038401 4.7 11
- 166 Stabilizing a hexagonal Ru₂C via Lifshitz transition under pressure. *Applied Physics Letters*, **2013**, 103, 251901 3.4 11
- 165 Pure and Li-doped NiTiH: Potential anode materials for Li-ion rechargeable batteries. *Applied Physics Letters*, **2013**, 103, 033902 3.4 11
- 164 Hydrogen as promoter and inhibitor of superionicity: A case study on Li-N-H systems. *Physical Review B*, **2010**, 82, 3.3 11
- 163 Theoretical investigation of xenon-hydrogen solids under pressure using ab initio DFT and GW calculations. *Physical Review B*, **2011**, 84, 3.3 11
- 162 Density Functional Theory Studies of Si₂BN Nanosheets as Anode Materials for Magnesium-Ion Batteries. *ACS Applied Nano Materials*, **2020**, 3, 9055-9063 5.6 11
- 161 Determining factors for the nano-biocompatibility of cobalt oxide nanoparticles: proximal discrepancy in intrinsic atomic interactions at differential vicinage. *Green Chemistry*, **2021**, 23, 3439-3458¹⁰ 11
- 160 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 3.8 10

159	Efficient Adsorption Characteristics of Pristine and Silver-Doped Graphene Oxide Towards Contaminants: A Potential Membrane Material for Water Purification?. <i>ChemPhysChem</i> , 2018 , 19, 2250-2257	3.2	10
158	Optical and electronic properties of nanosized BiTaO ₄ and BiNbO ₄ photocatalysts: Experiment and theory. <i>Physica Status Solidi (B): Basic Research</i> , 2014 , 251, 1034-1039	1.3	10
157	Pressure control of magnetic clusters in strongly inhomogeneous ferromagnetic chalcopyrites. <i>Scientific Reports</i> , 2015 , 5, 7720	4.9	10
156	Communication: Origin of the difference between carbon nanotube armchair and zigzag ends. <i>Journal of Chemical Physics</i> , 2014 , 140, 091102	3.9	10
155	Study of electronic and optical properties of BiTaO ₄ for photocatalysis. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2012 , 9, 1593-1596		10
154	Rational Design of 2D h-BAs Monolayer as Advanced Sulfur Host for High Energy Density LiS Batteries. <i>ACS Applied Energy Materials</i> , 2020 , 3, 7306-7317	6.1	10
153	Elucidating hydrogen storage properties of two-dimensional siligraphene (SiC ₈) monolayers upon selected metal decoration. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 5578-5587	5.8	10
152	Pressure-promoted highly-ordered Fe-doped-Ni ₂ B for effective oxygen evolution reaction and overall water splitting. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 6469-6475	13	10
151	Formation of Lightweight Ternary Polyhydrides and Their Hydrogen Storage Mechanism. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 1723-1730	3.8	10
150	Computational identification of efficient 2D Aluminium chalcogenides monolayers for optoelectronics and photocatalysts applications. <i>Applied Surface Science</i> , 2021 , 556, 149561	6.7	10
149	Manipulating carriers' spin polarization in the Heusler alloy Mn ₂ CoAl. <i>RSC Advances</i> , 2015 , 5, 73814-73819	197	9
148	Metal-functionalized 2D boron sulfide monolayer material enhancing hydrogen storage capacities. <i>Journal of Applied Physics</i> , 2020 , 127, 184305	2.5	9
147	Strain-Engineered Metal-Free h-B ₂ O Monolayer as a Mechanocatalyst for Photocatalysis and Improved Hydrogen Evolution Reaction. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 7884-7892	3.8	9
146	Rectifying behavior in twisted bilayer black phosphorus nanojunctions mediated through intrinsic anisotropy. <i>Nanoscale Advances</i> , 2020 , 2, 1493-1501	5.1	9
145	Room-temperature conversion of CuSe to CuAgSe nanoparticles to enhance the photocatalytic performance of their composites with TiO ₂ . <i>Dalton Transactions</i> , 2020 , 49, 3580-3591	4.3	9
144	Superior sensitivity of metal functionalized boron carbide (BC ₃) monolayer towards carbonaceous pollutants. <i>Applied Surface Science</i> , 2020 , 512, 145637	6.7	9
143	The High-Pressure Superconducting Phase of Arsenic. <i>Scientific Reports</i> , 2018 , 8, 3026	4.9	9
142	Improvement in the hydrogen desorption from MgH ₂ upon transition metals doping: A hybrid density functional calculations. <i>AIP Advances</i> , 2013 , 3, 102117	1.5	9

141	Emerging piezochromism in lead free alkaline earth chalcogenide perovskite AZrS3 (A = Mg, Ca, Sr and Ba) under pressure. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 16392-16403	7.1	9
140	Route to high-[Formula: see text] superconductivity of [Formula: see text] via strong bonding of boron-carbon compound at high pressure. <i>Scientific Reports</i> , 2020 , 10, 18090	4.9	9
139	Effect of electric field on optoelectronic properties of indiene monolayer for photoelectric nanodevices. <i>Scientific Reports</i> , 2019 , 9, 17300	4.9	9
138	Emergence of Si2BN Monolayer as Efficient HER Catalyst under Co-functionalization Influence. <i>ACS Applied Energy Materials</i> , 2019 , 2, 8441-8448	6.1	9
137	Anisotropic distortion and Lifshitz transition in Hf under pressure. <i>Physical Review B</i> , 2017 , 95,	3.3	8
136	Disorder-induced room temperature ferromagnetism in glassy chromites. <i>Scientific Reports</i> , 2014 , 4, 4686	4.9	8
135	Molecules versus Nanoparticles: Identifying a Reactive Molecular Intermediate in the Synthesis of Ternary Coinage Metal Chalcogenides. <i>Inorganic Chemistry</i> , 2020 , 59, 7727-7738	5.1	8
134	Exploring the Possibility of Phase Arsenic-Phosphorus Polymorph Monolayer as Anode Materials for Sodium-Ion Batteries. <i>Advanced Theory and Simulations</i> , 2020 , 3, 2000023	3.5	8
133	Theoretical Evidence behind Bifunctional Catalytic Activity in Pristine and Functionalized Al C Monolayers. <i>ChemPhysChem</i> , 2018 , 19, 148-152	3.2	8
132	Tuning electronic transport properties of zigzag graphene nanoribbons with silicon doping and phosphorus passivation. <i>AIP Advances</i> , 2018 , 8, 085123	1.5	8
131	Inquisitive Geometric Sites in h-BN Monolayer for Alkali Earth Metal Ion Batteries. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 19340-19346	3.8	8
130	New type of possible high-pressure polymorphism in NiAs minerals in planetary cores. <i>Physics and Chemistry of Minerals</i> , 2013 , 40, 183-193	1.6	8
129	Bromination-induced stability enhancement with a multivalley optical response signature in guanidinium [C(NH2)3]+-based hybrid perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 18561-18568	13	8
128	ELECTRONIC STATES IN INTERCALATION MATERIALS STUDIED BY ELECTROCHEMICAL TECHNIQUES. <i>Modern Physics Letters B</i> , 2006 , 20, 863-875	1.6	8
127	Li-decorated carbyne for hydrogen storage: charge induced polarization and van't Hoff hydrogen desorption temperature. <i>Sustainable Energy and Fuels</i> , 2020 , 4, 691-699	5.8	8
126	High pressure-induced distortion in face-centered cubic phase of thallium. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016 , 113, 11143-11147	11.5	8
125	Ultrahigh carrier mobility and light-harvesting performance of 2D penta-PdX2 monolayer. <i>Journal of Materials Science</i> , 2021 , 56, 3846-3860	4.3	8
124	8-16-4 graphyne: Square-lattice two-dimensional nodal line semimetal with a nontrivial topological Zak index. <i>Physical Review B</i> , 2021 , 103,	3.3	8

123	On the stability of single-walled carbon nanotubes and their binding strengths. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	7
122	Cotunnite-Structured Titanium Dioxide and the Hardest known Oxide. <i>High Pressure Research</i> , 2002 , 22, 429-433	1.6	7
121	Harnessing the unique properties of MXenes for advanced rechargeable batteries. <i>JPhys Energy</i> , 2021 , 3, 012005	4.9	7
120	Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in Two-Dimensional Thallium Selenide. <i>ACS Applied Energy Materials</i> , 2020 , 3, 9315-9325	6.1	7
119	Salt-assisted growth of monolayer MoS ₂ for high-performance hysteresis-free field-effect transistor. <i>Journal of Applied Physics</i> , 2021 , 129, 145106	2.5	7
118	Lithium-functionalized boron phosphide nanotubes (BPNTs) as an efficient hydrogen storage carrier. <i>International Journal of Hydrogen Energy</i> , 2021 , 46, 20586-20593	6.7	7
117	Degradation of Alzheimer's Amyloid- β by a Catalytically Inactive Insulin-Degrading Enzyme. <i>Journal of Molecular Biology</i> , 2021 , 433, 166993	6.5	7
116	The influence of edge structure on the optoelectronic properties of Si ₂ BN quantum dot. <i>Journal of Applied Physics</i> , 2019 , 126, 233104	2.5	7
115	Effect of Charge Injection on the Conducting Filament of Valence Change Anatase TiO Resistive Random Access Memory Device. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 1876-1884	6.4	7
114	Two-dimensional Janus Sn ₂ SSe and SnGeS ₂ semiconductors as strong absorber candidates for photovoltaic solar cells: First principles computations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 134, 114900	3	7
113	Highly Energetic and Stable Gadolinium/Bismuth Molybdate with a Fast Reactive Species, Redox Mechanism of Aqueous Electrolyte. <i>ACS Applied Energy Materials</i> , 2020 , 3, 12385-12399	6.1	6
112	Stability of a new cubic monoxide of Thorium under pressure. <i>Scientific Reports</i> , 2015 , 5, 13740	4.9	6
111	Crafting ferromagnetism in Mn-doped MgO surfaces with p-type defects. <i>Science and Technology of Advanced Materials</i> , 2014 , 15, 035008	7.1	6
110	Structural phase transition and metallization in compressed SrC ₂ . <i>Science Bulletin</i> , 2014 , 59, 5269-5271		6
109	Hybrid Density Functional and Molecular Dynamics Study of Promising Hydrogen Storage Materials: Double Metal Amidoboranes and Metal Amidoborane Ammoniates. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 17351-17359	3.8	6
108	Electronic structure of platinum at ultrahigh pressure. <i>High Pressure Research</i> , 1994 , 12, 161-170	1.6	6
107	Bain Deformation Mechanism and Lifshitz Transition in Magnesium under High Pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2021 , 258, 2000279	1.3	6
106	Stabilization and electronic topological transition of hydrogen-rich metal LiMoH under high pressures from first-principles predictions. <i>Scientific Reports</i> , 2021 , 11, 4079	4.9	6

105	Revealing the superlative electrochemical properties of o-B2N2 monolayer in Lithium/Sodium-ion batteries. <i>Nano Energy</i> , 2022 , 96, 107066	17.1	6
104	Hybrid-Functional Study of Native Defects and W/Mo-Doped in Monoclinic-Bismuth Vanadate. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 14508-14516	3.8	5
103	Highly Sensitive Gas Sensing Material for Environmentally Toxic Gases Based on Janus NbSeTe Monolayer. <i>Nanomaterials</i> , 2020 , 10,	5.4	5
102	Capacity enhancement of polyolithiated functionalized boron nitride nanotubes: an efficient hydrogen storage medium. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 15675-15682	3.6	5
101	Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. <i>Nanoscale Advances</i> , 2020 , 2, 2410-2421	5.1	5
100	Theoretical investigation of the structural, electronic, and thermodynamic properties of CdS1-xSex alloys. <i>Journal of Applied Physics</i> , 2018 , 123, 105103	2.5	5
99	Oxygen- and nitrogen-chemisorbed carbon nanostructures for Z-scheme photocatalysis applications. <i>Journal of Nanoparticle Research</i> , 2012 , 14, 1	2.3	5
98	Transport coefficients in diamond from ab-initio calculations. <i>Applied Physics Letters</i> , 2013 , 102, 092106	3.4	5
97	Resonant inelastic soft x-ray scattering at double core excitations in solid LiCl. <i>Physical Review B</i> , 2006 , 73,	3.3	5
96	Resonant Inelastic Soft X-Ray Scattering at Hollow Lithium States in Solid LiCl. <i>Physical Review Letters</i> , 2004 , 93,	7.4	5
95	Modified KBBF-like Material for Energy Storage Applications: ZnNiBO(OH) with Enhanced Cycle Life.. <i>ACS Applied Materials & Interfaces</i> , 2022 ,	9.5	5
94	Exploring the Degradation Behavior of Ce-Monazite in Water Solution through Adsorption and Penetration Kinetics. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 22173-22184	3.8	5
93	Tuning Hydrogen Storage Properties of Carbon Nanosheets through Selected Foreign Metal Functionalization. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 16827-16837	3.8	5
92	Carbon Nitride Monolayers as Efficient Immobilizers toward Lithium Selenides: Potential Applications in Lithium-Selenium Batteries. <i>ACS Applied Energy Materials</i> , 2021 , 4, 3891-3904	6.1	5
91	Modulation of 2D GaS/BTe vdW heterostructure as an efficient HER catalyst under external electric field influence. <i>Catalysis Today</i> , 2021 , 370, 14-25	5.3	5
90	Intrinsic atomic interaction at molecular proximal vicinity infer cellular biocompatibility of antibacterial nanopepper. <i>Nanomedicine</i> , 2021 , 16, 307-322	5.6	5
89	Electronic and Transport Properties of Bilayer Phosphorene Nanojunction: Effect of Paired Substitution Doping. <i>ACS Applied Electronic Materials</i> , 2021 , 3, 733-742	4	5
88	Ab Initio Screening of Doped Mg(AlH) Systems for Conversion-Type Lithium Storage. <i>Materials</i> , 2019 , 12,	3.5	4

87	Mapping the sodium intercalation mechanism, electrochemical properties and structural evolution in non-stoichiometric alluaudite $\text{Na}_{2+2x}\text{Fe}_2(\text{SO}_4)_3$ cathode materials. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 17446-17455	13	4
86	Van der Waals induced molecular recognition of canonical DNA nucleobases on a 2D GaS monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 6706-6715	3.6	4
85	New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT Studies. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 15646-15651	3.8	4
84	Atomistic study of promising catalyst and electrode material for memory capacitors: Platinum oxides. <i>Computational Materials Science</i> , 2013 , 79, 804-810	3.2	4
83	Ab initio study on pressure-induced change of effective Coulomb interaction in superconducting yttrium. <i>Applied Physics Letters</i> , 2010 , 96, 022510	3.4	4
82	Investigation on $\text{Ge}_5\text{Sb}_x\text{Te}_5$ phase-change materials by first-principles method. <i>Applied Physics A: Materials Science and Processing</i> , 2010 , 99, 961-964	2.6	4
81	H-H interaction and structural phase transition in Ti_3SnH_x . <i>Physical Review B</i> , 2002 , 66,	3.3	4
80	Eine Erklärung für die eigentliche Elementstruktur von Indium. <i>Angewandte Chemie</i> , 1999 , 111, 2155-2159	3.6	4
79	Tuning the Nanoparticle Interfacial Properties and Stability of the Core-Shell Structure in Zn-Doped $\text{NiMoO}_4/\text{AWO}$. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56116-56130	9.5	4
78	Molecular nanoinformatics approach assessing the biocompatibility of biogenic silver nanoparticles with channelized intrinsic steatosis and apoptosis. <i>Green Chemistry</i> ,	10	4
77	Antimonene Allotropes β and β' Phases as Promising Anchoring Materials for Lithium-Sulfur Batteries. <i>Energy & Fuels</i> , 2021 , 35, 9001-9009	4.1	4
76	Rare earth functionalization effect in optical response of ZnO nano clusters. <i>European Physical Journal D</i> , 2016 , 70, 1	1.3	4
75	Electric Field-Modulated Charge Transfer in Geometrically Tailored MoX_2/WX_2 (X = S, Se) Heterostructures. <i>Journal of Physical Chemistry C</i> ,	3.8	4
74	Role of relativity in high-pressure phase transitions of thallium. <i>Scientific Reports</i> , 2017 , 7, 42983	4.9	3
73	Magnetic order and phase diagram of magnetic alloy system: $\text{Mg}_x\text{Ni}_{1-x}\text{O}$ alloy. <i>Physica Status Solidi (B): Basic Research</i> , 2017 , 254, 1700085	1.3	3
72	Alloying in an Intercalation Host: Metal Titanium Niobates as Anodes for Rechargeable Alkali-Ion Batteries. <i>Chemistry - an Asian Journal</i> , 2018 , 13, 299-310	4.5	3
71	Investigation of the Factors That Dictate the Preferred Orientation of Lexitropsins in the Minor Groove of DNA. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 10423-10440	8.3	3
70	Studies of hypro-mellose (HPMC) functionalized ZnS:Mn fluorescent quantum dots. <i>Journal of Materials Science: Materials in Electronics</i> , 2017 , 28, 1931-1937	2.1	3

69	Nanoelectrodes: Enhanced DNA Sequencing Performance Through Edge-Hydrogenation of Graphene Electrodes (Adv. Funct. Mater. 14/2011). <i>Advanced Functional Materials</i> , 2011 , 21, 2602-2602	15.6	3
68	HYDROGEN STORAGE ENHANCEMENT VIA TRANSITION METAL DECORATION ON METAL ORGANIC FRAMEWORKS: A FIRST-PRINCIPLES STUDY. <i>Nano</i> , 2012 , 07, 1250044	1.1	3
67	Theoretical Prediction of a Bi-Doped β -Antimonene Monolayer as a Highly Efficient Photocatalyst for Oxygen Reduction and Overall Water Splitting. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 56234-56234	9.5	3
66	Temperature-Dependent Cationic Doping-Driven Phonon Dynamics Investigation in CdO Thin Films Using Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 21818-21828	3.8	3
65	Dimensionality effects in high-performance thermoelectric materials: Computational and experimental progress in energy harvesting applications. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , e1547	7.9	3
64	Local electrocatalytic activity of PtRu supported on nitrogen-doped carbon nanotubes towards methanol oxidation by scanning electrochemical microscopy. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 21291-21301	13	3
63	Nanolayered MAX Phases from Ab Initio Calculations	199-204	3
62	Janus Aluminum Oxysulfide Al ₂ OS: A promising 2D direct semiconductor photocatalyst with strong visible light harvesting. <i>Applied Surface Science</i> , 2022 , 589, 152997	6.7	3
61	Unsaturated surface in CO saturation. <i>Surface and Interface Analysis</i> , 2017 , 49, 892-897	1.5	2
60	Carbides-anti-perovskites Mn ₃ (Sn, Zn)C: Potential candidates for an application in magnetic refrigeration. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 124, 114317	3	2
59	Theoretical aspects in structural distortion and the electronic properties of lithium peroxide under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 9488-9497	3.6	2
58	Defect Thermodynamics in Nonstoichiometric Alluaudite-Based Polyanionic Materials for Na-Ion Batteries. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 32856-32868	9.5	2
57	Phase stability and superconductivity of strontium under pressure. <i>Applied Physics Letters</i> , 2012 , 101, 052604	3.4	2
56	Magnetoresistance and Hall-effect measurements of Ni thin films. <i>Journal of Applied Physics</i> , 2005 , 97, 083902	2.5	2
55	Binding and optical characteristics of polycyclic aromatic hydrocarbons and their nitroderivatives adsorbed on the C ₃ N monolayer. <i>New Journal of Chemistry</i> , 2022 , 46, 2245-2258	3.6	2
54	Emerging piezochromism in transparent lead free perovskite Rb ₃ X ₂ I ₉ (X = Sb, Bi) under compression: A comparative theoretical insight. <i>Journal of Applied Physics</i> , 2020 , 128, 045102	2.5	2
53	From Monolayers to Nanotubes: Toward Catalytic Transition-Metal Dichalcogenides for Hydrogen Evolution Reaction. <i>Energy & Fuels</i> , 2021 , 35, 6282-6288	4.1	2
52	Design of Continuous Transport of the Droplet by the Contact-Boiling Regime. <i>Langmuir</i> , 2021 , 37, 553-560	5.0	2

51	Large-Scale Fabrication of Wettability-Controllable Coatings for Optimizing Condensate Transfer Ability. <i>Langmuir</i> , 2021 , 37, 2476-2484	4	2
50	High-temperature superconductor of sodalite-like clathrate hafnium hexahydride. <i>Scientific Reports</i> , 2021 , 11, 16403	4.9	2
49	Potential SiX (X = N, P, As, Sb, Bi) homo-bilayers for visible-light photocatalyst applications. <i>Catalysis Science and Technology</i> , 2021 , 11, 4996-5013	5.5	2
48	Two-Dimensional Bismuthene Nanosheets for Selective Detection of Toxic Gases. <i>ACS Applied Nano Materials</i> , 2022 , 5, 2984-2993	5.6	2
47	Dynamical modeling of miR-34a, miR-449a, and miR-16 reveals numerous DDR signaling pathways regulating senescence, autophagy, and apoptosis in HeLa cells.. <i>Scientific Reports</i> , 2022 , 12, 4911	4.9	2
46	Structural Evolution of AlN Nanoclusters and the Elemental Chemisorption Characteristics: Atomistic Insight. <i>Nanomaterials</i> , 2019 , 9,	5.4	1
45	Mechanical and electronic properties of van der Waals layered hcp PdH. <i>Scientific Reports</i> , 2020 , 10, 8037.	4.9	1
44	2D monolayer boron sulfide as an efficient material for optical nanodevices 2020 ,		1
43	HfS2 and TiS2 Monolayers with Adsorbed C, N, P Atoms: A First Principles Study. <i>Catalysts</i> , 2020 , 10, 94	4	1
42	Chemical Bonding of Unique CO on Fe(100). <i>Journal of Physical Chemistry C</i> , 2018 , 122, 9062-9074	3.8	1
41	Time dependent DFT investigation of the optical response in pristine and Gd doped Al2O3. <i>RSC Advances</i> , 2016 , 6, 72537-72543	3.7	1
40	High-Pressure Phase Transition of ZnO Nanorods Using Density Functional Theory. <i>Integrated Ferroelectrics</i> , 2014 , 156, 122-128	0.8	1
39	Elucidating the reaction pathway of crystalline multi-metal borides for highly efficient oxygen-evolving electrocatalysts. <i>Journal of Materials Chemistry A</i> , 2022 , 10, 1569-1578	13	1
38	Contact electrification through interfacial charge transfer: a mechanistic viewpoint on solid-liquid interfaces. <i>Nanoscale Advances</i> , 2022 , 4, 884-893	5.1	1
37	Fabrication of BP2T functionalized graphene non-covalent π - π stacking interactions for enhanced ammonia detection.. <i>RSC Advances</i> , 2021 , 11, 35982-35987	3.7	1
36	Mechanistic Understanding of the Interactions and Pseudocapacitance of Multi-Electron Redox Organic Molecules Sandwiched between MXene Layers. <i>Advanced Electronic Materials</i> , 2021 , 7, 2001202	6.4	1
35	Mechanism of formaldehyde and formic acid formation on (101)-TiO2@Cu4 systems through CO2 hydrogenation. <i>Sustainable Energy and Fuels</i> , 2021 , 5, 564-574	5.8	1
34	Large-Scale Screening of Interface Parameters in the WC/W System Using Classical Force Field and First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 3631-3639	3.8	1

33	Understanding carbon dioxide capture on metal-organic frameworks from first-principles theory: The case of MIL-53(X), with X = Fe, Al, and Cu. <i>Journal of Chemical Physics</i> , 2021 , 155, 024701	3.9	1
32	Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. <i>Journal of Computational Chemistry</i> , 2021 , 42, 1944-1958	3.5	1
31	High-Specific-Capacity and High-Performing Post-Lithium-Ion Battery Anode over 2D Black Arsenic Phosphorus. <i>ACS Applied Energy Materials</i> , 2021 , 4, 7900-7910	6.1	1
30	Exploring the relationship between Ln leaching and Ln O binding energy in monazite (Nd, Sm, Eu). <i>Journal of the American Ceramic Society</i> , 2022 , 105, 553	3.8	1
29	MXene binder stabilizes pseudocapacitance of conducting polymers. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20356-20361	13	1
28	Strain-mediated ferromagnetism and low-field magnetic reversal in Co doped monolayer [Formula: see text].. <i>Scientific Reports</i> , 2022 , 12, 2593	4.9	1
27	Strain modulating electronic band gaps and SQ efficiencies of semiconductor 2D PdQ (Q = S, Se) monolayer.. <i>Scientific Reports</i> , 2022 , 12, 2964	4.9	1
26	2D Janus and non-Janus diamanes with an in-plane negative Poisson's ratio for energy applications. <i>Materials Today Advances</i> , 2022 , 14, 100225	7.4	1
25	Antibodies Against Phosphorylcholine Among 60-Year-Olds: Clinical Role and Simulated Interactions.. <i>Frontiers in Cardiovascular Medicine</i> , 2022 , 9, 809007	5.4	1
24	Bifunctional Catalytic Activity of 2D Boron Monochalcogenides BX (X = S, Se, Te). <i>Materials Today Energy</i> , 2022 , 101026	7	1
23	Recent Advancements in Nontoxic Halide Perovskites: Beyond Divalent Composition Space.. <i>ACS Omega</i> , 2021 , 6, 33240-33252	3.9	0
22	Asymmetry-Induced Redistribution in Sn(IV)Ti(IV) Hetero-Bimetallic Alkoxide Precursors and Its Impact on Thin-Film Deposition by MetalOrganic Chemical Vapor Deposition. <i>Crystal Growth and Design</i> ,	3.5	0
21	Pressure-induced order-disorder transitions in InS: an experimental and theoretical study of structural and vibrational properties. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 23625-23642	3.6	0
20	Ultrathin nanowire PdX ₂ (X = P, As): stability, electronic transport and thermoelectric properties. <i>New Journal of Chemistry</i> , 2020 , 44, 15617-15624	3.6	0
19	Hydrogenation and oxidation enhances the thermoelectric performance of Si ₂ BN monolayer. <i>New Journal of Chemistry</i> , 2021 , 45, 3892-3900	3.6	0
18	Correlation between reduced dielectric loss and charge migration kinetics in NdFeO ₃ -modified Ba _{0.7} Sr _{0.3} TiO ₃ ceramics. <i>Journal of Materials Science: Materials in Electronics</i> , 2021 , 32, 24910	2.1	0
17	Metallic one-dimensional heterostructure for gas molecule sensing. <i>Scientific Reports</i> , 2021 , 11, 433	4.9	0
16	Stabilizing superconductivity of ternary metal pentahydride [Formula: see text] via electronic topological transitions under high pressure from first principles evolutionary algorithm.. <i>Scientific Reports</i> , 2022 , 12, 6700	4.9	0

- 15 Poisonous Vapor Adsorption on Pure and Modified Aluminum Nitride Nanosheet for Environmental Safety: A DFT Exploration. *Sustainability*, **2020**, 12, 10097 3.6
- 14 Evaluating bulk Nb₂O₂F₃ for Li-battery electrode applications. *Physical Chemistry Chemical Physics*, **2016**, 18, 3530-5 3.6
- 13 Improvement in Hydrogen Desorption from δ and ϵ -MgH₂ upon Transition-Metal Doping. *ChemPhysChem*, **2015**, 16, 2481-2481 3.2
- 12 Electronic Structure and High-Pressure Behavior of Solids **2010**, 269-290
- 11 High-pressure structural transitions in Cm and Am_{0.5}Cm_{0.5} binary alloy. *High Pressure Research*, **2006**, 26, 377-381 1.6
- 10 High Pressure structural transitions in Cm metal. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1
- 9 Theoretical study of protactinium at high pressure. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1
- 8 Phase transitions in Am_{0.5}Cm_{0.5} binary alloy. *Materials Research Society Symposia Proceedings*, **2005**, 893, 1
- 7 High pressure studies of sodium and silver halides. *High Pressure Research*, **2000**, 18, 131-138 1.6
- 6 First Principles Simulations of Phase Stability in Stoichiometric and Doped LiMnO₂. *Materials Research Society Symposia Proceedings*, **2001**, 677, 4161
- 5 No-Carbon 2D Anode Materials for Next-Generation Batteries **2021**, 1-14
- 4 Data-Driven Machine Learning Approaches for Advanced Battery Modeling **2021**, 1-18
- 3 MXene-Based 2D Anode Materials for Next-Generation Batteries **2021**, 1-20
- 2 Coexisting commensurate and incommensurate charge ordered phases in CoO. *Scientific Reports*, **2021**, 11, 19415 4.9
- 1 Preparation and properties of situ-sintered SiC ceramics aided by ZnO-Al₂O₃-CaO. *Journal of Alloys and Compounds*, **2022**, 890, 161854 5.7