

Petr Lazar

List of Publications by Year in descending order

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77
papers

3,667
citations

136885

32
h-index

133188

59
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78
all docs

78
docs citations

78
times ranked

5914
citing authors

#	ARTICLE	IF	CITATIONS
1	Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment. <i>Applied Surface Science</i> , 2022, 587, 152839.	3.1	8
2	Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Single-Atom Catalysts. <i>Advanced Materials Interfaces</i> , 2021, 8, 2001392.	1.9	6
3	Vanadium Dopants: A Boon or a Bane for Molybdenum Dichalcogenides-Based Electrocatalysis Applications. <i>Advanced Functional Materials</i> , 2021, 31, 2009083.	7.8	14
4	1D Coordination π -Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 439-445.	7.2	23
5	1D Coordination π -Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. <i>Angewandte Chemie</i> , 2021, 133, 443-449.	1.6	0
6	Rhenium Doping of Layered Transition-Metal Diselenides Triggers Enhancement of Photoelectrochemical Activity. <i>ACS Nano</i> , 2021, 15, 2374-2385.	7.3	19
7	Silver Covalently Bound to Cyanographene Overcomes Bacterial Resistance to Silver Nanoparticles and Antibiotics. <i>Advanced Science</i> , 2021, 8, 2003090.	5.6	27
8	Two-Dimensional Functionalized Germananes as Photoelectrocatalysts. <i>ACS Nano</i> , 2021, 15, 11681-11693.	7.3	25
9	Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene. <i>Applied Surface Science</i> , 2021, 565, 150382.	3.1	2
10	Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 61751-61757.	4.0	9
11	Mechanistic Insight into the Limiting Factors of Graphene-Based Environmental Sensors. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 39764-39771.	4.0	13
12	Atomic-Scale Edge Morphology, Stability, and Oxidation of Single-Layer $2H-TaS_2$. <i>ChemPlusChem</i> , 2020, 85, 2557-2564.	1.3	5
13	Surface Energy of Black Phosphorus Alloys with Arsenic. <i>ChemNanoMat</i> , 2020, 6, 821-826.	1.5	6
14	Oxidation of metallic two-dimensional transition metal dichalcogenides: $1T-MoS_2$ and $1T-TaS_2$. <i>2D Materials</i> , 2020, 7, 045005.	2.0	15
15	Acetonitrile-assisted exfoliation of layered grey and black arsenic: contrasting properties. <i>Nanoscale Advances</i> , 2020, 2, 1282-1289.	2.2	21
16	Tailoring Electronic and Magnetic Properties of Graphene by Phosphorus Doping. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 34074-34085.	4.0	20
17	Atomic-Scale Charge Distribution Mapping of Single Substitutional p- and n-Type Dopants in Graphene. <i>ACS Sustainable Chemistry and Engineering</i> , 2020, 8, 3437-3444.	3.2	13
18	Positive and Negative Effects of Dopants toward Electrocatalytic Activity of MoS_2 and WS_2 : Experiments and Theory. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 20383-20392.	4.0	38

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19	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. <i>Applied Materials Today</i> , 2019, 17, 112-122.	2.3	25
20	Microwave Energy Drives "Off" Spin-Switch Behavior in Nitrogen-Doped Graphene. <i>Advanced Materials</i> , 2019, 31, e1902587.	11.1	15
21	Chalcogenide vacancies drive the electrocatalytic performance of rhenium dichalcogenides. <i>Nanoscale</i> , 2019, 11, 14684-14690.	2.8	15
22	Identification of Two-Dimensional FeO ₂ Termination of Bulk Hematite $\sqrt{3}\times\sqrt{3}$ (0001) Surface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14312-14318.	1.5	5
23	Surface termination of MgB ₂ unveiled by a combination of adsorption experiments and theoretical calculations. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7313-7320.	1.3	3
24	Spectroscopic Fingerprints of Graphitic, Pyrrolic, Pyridinic, and Chemisorbed Nitrogen in N-Doped Graphene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 10695-10702.	1.5	181
25	Role of the puckered anisotropic surface in the surface and adsorption properties of black phosphorus. <i>Nanoscale</i> , 2018, 10, 8979-8988.	2.8	27
26	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. <i>Nanoscale</i> , 2018, 10, 4696-4707.	2.8	55
27	Ta ₃ Nanofibers: Layered Trichalcogenide for High-Performance Electronic and Sensing Devices. <i>ACS Nano</i> , 2018, 12, 464-473.	7.3	30
28	Role of the Edge Properties in the Hydrogen Evolution Reaction on MoS ₂ . <i>Chemistry - A European Journal</i> , 2017, 23, 4863-4869.	1.7	31
29	High-Yield Alkylation and Arylation of Graphene via Grignard Reaction with Fluorographene. <i>Chemistry of Materials</i> , 2017, 29, 926-930.	3.2	64
30	Functional Nanosheet Synthons by Covalent Modification of Transition-Metal Dichalcogenides. <i>Chemistry of Materials</i> , 2017, 29, 2066-2073.	3.2	56
31	2H \rightarrow 1T Phase Engineering of Layered Tantalum Disulfides in Electrocatalysis: Oxygen Reduction Reaction. <i>Chemistry - A European Journal</i> , 2017, 23, 8082-8091.	1.7	33
32	Interaction of the Helium, Hydrogen, Air, Argon, and Nitrogen Bubbles with Graphite Surface in Water. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 17517-17525.	4.0	13
33	The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9891-9896.	7.2	159
34	Universal Method for Large-Scale Synthesis of Layered Transition Metal Dichalcogenides. <i>Chemistry - A European Journal</i> , 2017, 23, 10177-10186.	1.7	22
35	Is Single Layer MoS ₂ Stable in the Air?. <i>Chemistry - A European Journal</i> , 2017, 23, 13233-13239.	1.7	80
36	Surface properties of MoS ₂ probed by inverse gas chromatography and their impact on electrocatalytic properties. <i>Nanoscale</i> , 2017, 9, 19236-19244.	2.8	19

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37	The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents. <i>Angewandte Chemie</i> , 2017, 129, 10023-10028.	1.6	26
38	Layered Transition-Metal Ditellurides in Electrocatalytic Applications—Contrasting Properties. <i>ACS Catalysis</i> , 2017, 7, 5706-5716.	5.5	50
39	Direct mapping of chemical oxidation of individual graphene sheets through dynamic force measurements at the nanoscale. <i>Nanoscale</i> , 2017, 9, 119-127.	2.8	21
40	Layered Platinum Dichalcogenides (PtS ₂ , PtSe ₂ , and PtTe ₂) Electrocatalysis: Monotonic Dependence on the Chalcogen Size. <i>Advanced Functional Materials</i> , 2016, 26, 4306-4318.	7.8	228
41	Electrocatalysis of layered Group 5 metallic transition metal dichalcogenides (MX ₂ , M = Tj ETQq1 1 0,784314 rgBT / Overl	5.2	218
42	Layered SnS versus SnS ₂ : Valence and Structural Implications on Electrochemistry and Clean Energy Electrocatalysis. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24098-24111.	1.5	85
43	Organic adsorbates have higher affinities to fluorographene than to graphene. <i>Applied Materials Today</i> , 2016, 5, 142-149.	2.3	43
44	Structure, dynamical stability, and electronic properties of phases in TaS ₂ from a high-level quantum mechanical calculation. <i>Physical Review B</i> , 2015, 92, .	1.1	34
45	Negative thermal expansion of ScF ₃ Insights from density-functional molecular dynamics in the isothermal-isobaric ensemble. <i>Physical Review B</i> , 2015, 92, .	1.1	34
46	Accurate surface energies from first principles. <i>Physical Review B</i> , 2015, 91, .	1.1	35
47	Fluorographene: Dichlorocarbene-Functionalized Fluorographene: Synthesis and Reaction Mechanism (Small 31/2015). <i>Small</i> , 2015, 11, 3789-3789.	5.2	2
48	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1430-1434.	2.1	90
49	Dichlorocarbene-Functionalized Fluorographene: Synthesis and Reaction Mechanism. <i>Small</i> , 2015, 11, 3790-3796.	5.2	32
50	The surface and structural properties of graphite fluoride. <i>Carbon</i> , 2015, 94, 804-809.	5.4	53
51	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isothermic Adsorption Enthalpies. <i>Journal of Physical Chemistry C</i> , 2015, 119, 20535-20543.	1.5	31
52	The nature of high surface energy sites in graphene and graphite. <i>Carbon</i> , 2014, 73, 448-453.	5.4	38
53	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. <i>Journal of Physical Chemistry C</i> , 2014, 118, 13817-13825.	1.5	114
54	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 20818-20827.	1.3	10

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55	Chemical nature of boron and nitrogen dopant atoms in graphene strongly influences its electronic properties. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14231-14235.	1.3	86
56	Spin-Crossing in an Organometallic Pt-Benzene Complex. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1461-1468.	2.3	19
57	Adsorption of Small Organic Molecules on Graphene. <i>Journal of the American Chemical Society</i> , 2013, 135, 6372-6377.	6.6	407
58	Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions. <i>ACS Nano</i> , 2013, 7, 1646-1651.	7.3	73
59	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3670-3676.	2.3	39
60	Interaction of Graphene and Arenes with Noble Metals. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14151-14162.	1.5	45
61	Dissociation of Water at Iron Surfaces: Generalized Gradient Functional and Range-Separated Hybrid Functional Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25470-25477.	1.5	29
62	Structure, bonding, and possible superhardness of CrB ₄ . <i>Physical Review B</i> , 2012, 85, .	1.1	154
63	The Nature of the Binding of Au, Ag, and Pd to Benzene, Coronene, and Graphene: From Benchmark CCSD(T) Calculations to Plane-Wave DFT Calculations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3743-3755.	2.3	100
64	Temperature-induced martensitic phase transitions in gum-metal approximants: First-principles investigations for Ti ₃ Nb. <i>Physical Review B</i> , 2011, 84, .	1.1	41
65	Unveiling the atomic and electronic structure of the VN/MgO interface. <i>Physical Review B</i> , 2010, 82, .	1.1	3
66	First-principles modeling of hardness in transition-metal diborides. <i>Physical Review B</i> , 2009, 80, .	1.1	52
67	Mechanical properties of superhard BC ₅ . <i>Applied Physics Letters</i> , 2009, 94, .	1.5	21
68	Ductility and magnetism: An ab-initio study of NiAl-Fe and NiAl-Mn alloys. <i>Intermetallics</i> , 2009, 17, 675-679.	1.8	21
69	N-K electron energy-loss near-edge structures for TiN/VN layers: an ab initio and experimental study. <i>Analytical and Bioanalytical Chemistry</i> , 2008, 390, 1447-1453.	1.9	14
70	Interface structure of epitaxial (111) VN films on (111) MgO substrates. <i>Thin Solid Films</i> , 2008, 517, 1177-1181.	0.8	15
71	Cleavage fracture of a crystal: Density functional theory calculations based on a model which includes structural relaxations. <i>Physical Review B</i> , 2008, 78, .	1.1	62
72	Density functional theory study of ternary V-Cr-N compounds. <i>Physical Review B</i> , 2008, 78, .	1.1	11

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73	Ab initio study of tension-shear coupling in NiAl. Physical Review B, 2007, 75, .	1.1	20
74	Density functional theory applied to $N \langle \mathbf{m} \rangle \cdot V$ $Ti \langle \mathbf{m} \rangle \cdot N$ multilayers. Physical Review B, 2007, 76, .	1.1	71
75	Combined ab-initio and N-K, Ti-L _{2,3} , V-L _{2,3} electron energy-loss near edge structure studies for TiN and VN films. International Journal of Materials Research, 2007, 98, 1060-1065.	0.1	5
76	Ab initio study of the mechanical properties of NiAl microalloyed by X=Cr, Mo, Ti, Ga. Physical Review B, 2006, 73, .	1.1	96
77	Correlating elasticity and cleavage. Applied Physics Letters, 2005, 87, 261910.	1.5	36