Petr Lazar

List of Publications by Year
in descending order

77 papers	3,667 citations	136885 32 h-index	133188 59 g-index
78 all docs	78 docs citations	78 times ranked	5914 citing authors

#	Article	IF	Citations
1	Adsorption of Small Organic Molecules on Graphene. Journal of the American Chemical Society, 2013, 135, 6372-6377.	6.6	407
2	Layered Platinum Dichalcogenides (PtS₂, PtSe₂, and PtTe₂) Electrocatalysis: Monotonic Dependence on the Chalcogen Size. Advanced Functional Materials, 2016, 26, 4306-4318.	7.8	228
3	Electrocatalysis of layered Group 5 metallic transition metal dichalcogenides (MX₂, M =) Tj ETQq1 1 0.784314 rgBT /Ove	5.2	218
4	Spectroscopic Fingerprints of Graphitic, Pyrrolic, Pyridinic, and Chemisorbed Nitrogen in N-Doped Graphene. Journal of Physical Chemistry C, 2019, 123, 10695-10702.	1.5	181
5	The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents. Angewandte Chemie - International Edition, 2017, 56, 9891-9896.	7.2	159
6	Structure, bonding, and possible superhardness of CrB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	154
7	Anaerobic Reaction of Nanoscale Zerovalent Iron with Water: Mechanism and Kinetics. Journal of Physical Chemistry C, 2014, 118, 13817-13825.	1.5	114
8	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. Journal of Chemical Theory and Computation, 2011, 7, 3743-3755.	2.3	100
9	Ab initiostudy of the mechanical properties ofNiAlmicroalloyed byX=Cr,Mo,Ti,Ga. Physical Review B, 2006, 73, .	1.1	96
10	Reactivity of Fluorographene: A Facile Way toward Graphene Derivatives. Journal of Physical Chemistry Letters, 2015, 6, 1430-1434.	2.1	90
11	Chemical nature of boron and nitrogen dopant atoms in graphene strongly influences its electronic properties. Physical Chemistry Chemical Physics, 2014, 16, 14231-14235.	1.3	86
12	Layered SnS versus SnS₂: Valence and Structural Implications on Electrochemistry and Clean Energy Electrocatalysis. Journal of Physical Chemistry C, 2016, 120, 24098-24111.	1.5	85
13	Is Single Layer MoS₂ Stable in the Air?. Chemistry - A European Journal, 2017, 23, 13233-13239.	1.7	80
14	Quantification of the Interaction Forces between Metals and Graphene by Quantum Chemical Calculations and Dynamic Force Measurements under Ambient Conditions. ACS Nano, 2013, 7, 1646-1651.	7.3	73
15	Density functional theory applied to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">V</mml:mi><mml:mi mathvariant="normal">N</mml:mi><mml:mo>â^•</mml:mo><mml:mi mathvariant="normal">Ti</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>multilayers. Physical Review B, 2007, 76, .	1.1	71
16	High-Yield Alkylation and Arylation of Graphene via Grignard Reaction with Fluorographene. Chemistry of Materials, 2017, 29, 926-930.	3.2	64
17	Cleavage fracture of a crystal: Density functional theory calculations based on a model which includes structural relaxations. Physical Review B, 2008, 78, .	1.1	62
18	Functional Nanosheet Synthons by Covalent Modification of Transition-Metal Dichalcogenides. Chemistry of Materials, 2017, 29, 2066-2073.	3.2	56

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19	Reactivity of fluorographene is triggered by point defects: beyond the perfect 2D world. Nanoscale, 2018, 10, 4696-4707.	2.8	55
20	The surface and structural properties of graphite fluoride. Carbon, 2015, 94, 804-809.	5.4	53
21	First-principles modeling of hardness in transition-metal diborides. Physical Review B, 2009, 80, .	1.1	52
22	Layered Transition-Metal Ditellurides in Electrocatalytic Applicationsâ€"Contrasting Properties. ACS Catalysis, 2017, 7, 5706-5716.	5.5	50
23	Interaction of Graphene and Arenes with Noble Metals. Journal of Physical Chemistry C, 2012, 116, 14151-14162.	1.5	45
24	Organic adsorbates have higher affinities to fluorographene than to graphene. Applied Materials Today, 2016, 5, 142-149.	2.3	43
25	Temperature-induced martensitic phase transitions in gum-metal approximants: First-principles investigations for Ti<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Nb. Physical Review B, 2011, 84, .	1.1	41
26	Structure, dynamical stability, and electronic properties of phases in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>TaS</mml:mtext><mml:mn>2</mml:mn></mml:msub a high-level quantum mechanical calculation. Physical Review B, 2015, 92, .	1.1	40
27	Random Phase Approximation in Surface Chemistry: Water Splitting on Iron. Journal of Chemical Theory and Computation, 2013, 9, 3670-3676.	2.3	39
28	The nature of high surface energy sites in graphene and graphite. Carbon, 2014, 73, 448-453.	5.4	38
29	Positive and Negative Effects of Dopants toward Electrocatalytic Activity of MoS₂ and WS₂: Experiments and Theory. ACS Applied Materials & Interfaces, 2020, 12, 20383-20392.	4.0	38
30	Correlating elasticity and cleavage. Applied Physics Letters, 2005, 87, 261910.	1.5	36
31	Accurate surface energies from first principles. Physical Review B, 2015, 91, .	1.1	35
32	Negative thermal expansion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScF</mml:mi><mml:mn>3</mml:mn></mml:msub></mml Insights from density-functional molecular dynamics in the isothermal-isobaric ensemble. Physical Review B, 2015, 92, .	1.1	34
33	2Hâ†'1T Phase Engineering of Layered Tantalum Disulfides in Electrocatalysis: Oxygen Reduction Reaction. Chemistry - A European Journal, 2017, 23, 8082-8091.	1.7	33
34	Dichlorocarbeneâ€Functionalized Fluorographene: Synthesis and Reaction Mechanism. Small, 2015, 11, 3790-3796.	5.2	32
35	Interplay between Ethanol Adsorption to High-Energy Sites and Clustering on Graphene and Graphite Alters the Measured Isosteric Adsorption Enthalpies. Journal of Physical Chemistry C, 2015, 119, 20535-20543.	1.5	31
36	Role of the Edge Properties in the Hydrogen Evolution Reaction on MoS₂. Chemistry - A European Journal, 2017, 23, 4863-4869.	1.7	31

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37	TaS₃ Nanofibers: Layered Trichalcogenide for High-Performance Electronic and Sensing Devices. ACS Nano, 2018, 12, 464-473.	7.3	30
38	Dissociation of Water at Iron Surfaces: Generalized Gradient Functional and Range-Separated Hybrid Functional Study. Journal of Physical Chemistry C, 2012, 116, 25470-25477.	1.5	29
39	Role of the puckered anisotropic surface in the surface and adsorption properties of black phosphorus. Nanoscale, 2018, 10, 8979-8988.	2.8	27
40	Silver Covalently Bound to Cyanographene Overcomes Bacterial Resistance to Silver Nanoparticles and Antibiotics. Advanced Science, 2021, 8, 2003090.	5.6	27
41	The Covalent Functionalization of Layered Black Phosphorus by Nucleophilic Reagents. Angewandte Chemie, 2017, 129, 10023-10028.	1.6	26
42	Intrinsic photoluminescence of amine-functionalized graphene derivatives for bioimaging applications. Applied Materials Today, 2019, 17, 112-122.	2.3	25
43	Two-Dimensional Functionalized Germananes as Photoelectrocatalysts. ACS Nano, 2021, 15, 11681-11693.	7.3	25
44	1D Coordination Ï€â€“d Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. Angewandte Chemie - International Edition, 2021, 60, 439-445.	7.2	23
45	Universal Method for Largeâ€Scale Synthesis of Layered Transition Metal Dichalcogenides. Chemistry - A European Journal, 2017, 23, 10177-10186.	1.7	22
46	Mechanical properties of superhard BC5. Applied Physics Letters, 2009, 94, .	1.5	21
47	Ductility and magnetism: An ab-initio study of NiAlâ€“Fe and NiAlâ€“Mn alloys. Intermetallics, 2009, 17, 675-679.	1.8	21
48	Direct mapping of chemical oxidation of individual graphene sheets through dynamic force measurements at the nanoscale. Nanoscale, 2017, 9, 119-127.	2.8	21
49	Acetonitrile-assisted exfoliation of layered grey and black arsenic: contrasting properties. Nanoscale Advances, 2020, 2, 1282-1289.	2.2	21
50	Ab initiostudy of tension-shear coupling in NiAl. Physical Review B, 2007, 75, .	1.1	20
51	Tailoring Electronic and Magnetic Properties of Graphene by Phosphorus Doping. ACS Applied Materials & Interfaces, 2020, 12, 34074-34085.	4.0	20
52	Spin-Crossing in an Organometallic Ptâ€“Benzene Complex. Journal of Chemical Theory and Computation, 2013, 9, 1461-1468.	2.3	19
53	Surface properties of MoS₂ probed by inverse gas chromatography and their impact on electrocatalytic properties. Nanoscale, 2017, 9, 19236-19244.	2.8	19
54	Rhenium Doping of Layered Transition-Metal Diselenides Triggers Enhancement of Photoelectrochemical Activity. ACS Nano, 2021, 15, 2374-2385.	7.3	19

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55	Interface structure of epitaxial (111) VN films on (111) MgO substrates. Thin Solid Films, 2008, 517, 1177-1181.	0.8	15
56	Microwave Energy Drives â€œOnâ€“Offâ€“Onâ€•Spinâ€Switch Behavior in Nitrogenâ€Doped Graphene. Advanced Materials, 2019, 31, e1902587.	11.1	15
57	Chalcogenide vacancies drive the electrocatalytic performance of rhenium dichalcogenides. Nanoscale, 2019, 11, 14684-14690.	2.8	15
58	Oxidation of metallic two-dimensional transition metal dichalcogenides: 1T-MoS₂ and 1T-TaS₂. 2D Materials, 2020, 7, 045005.	2.0	15
59	N-K electron energy-loss near-edge structures for TiN/VN layers: an ab initio and experimental study. Analytical and Bioanalytical Chemistry, 2008, 390, 1447-1453.	1.9	14
60	Vanadium Dopants: A Boon or a Bane for Molybdenum Dichalcogenidesâ€Based Electrocatalysis Applications. Advanced Functional Materials, 2021, 31, 2009083.	7.8	14
61	Interaction of the Helium, Hydrogen, Air, Argon, and Nitrogen Bubbles with Graphite Surface in Water. ACS Applied Materials & Interfaces, 2017, 9, 17517-17525.	4.0	13
62	Mechanistic Insight into the Limiting Factors of Graphene-Based Environmental Sensors. ACS Applied Materials & Interfaces, 2020, 12, 39764-39771.	4.0	13
63	Atomic-Scale Charge Distribution Mapping of Single Substitutional p- and n-Type Dopants in Graphene. ACS Sustainable Chemistry and Engineering, 2020, 8, 3437-3444.	3.2	13
64	Density functional theory study of ternary V-Cr-N compounds. Physical Review B, 2008, 78, .	1.1	11
65	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. Physical Chemistry Chemical Physics, 2014, 16, 20818-20827.	1.3	10
66	Graphene Field Effect Transistors: A Sensitive Platform for Detecting Sarin. ACS Applied Materials & Interfaces, 2021, 13, 61751-61757.	4.0	9
67	Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment. Applied Surface Science, 2022, 587, 152839.	3.1	8
68	Surface Energy of Black Phosphorus Alloys with Arsenic. ChemNanoMat, 2020, 6, 821-826.	1.5	6
69	Anchoring of Transition Metals to Graphene Derivatives as an Efficient Approach for Designing Singleâ€Atom Catalysts. Advanced Materials Interfaces, 2021, 8, 2001392.	1.9	6
70	Combined ab-initio and N-K, Ti-L₂,3, V-L₂,3 electron energy-loss near edge structure studies for TiN and VN films. International Journal of Materials Research, 2007, 98, 1060-1065.	0.1	5
71	Identification of Two-Dimensional FeO₂ Termination of Bulk Hematite Î±-Fe₂O₃(0001) Surface. Journal of Physical Chemistry C, 2019, 123, 14312-14318.	1.5	5
72	Atomicâ€Scale Edge Morphology, Stability, and Oxidation of Singleâ€Layer 2Hâ€TaS₂. ChemPlusChem, 2020, 85, 2557-2564.	1.3	5

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73	Unveiling the atomic and electronic structure of the VN/MgO interface. Physical Review B, 2010, 82, .	1.1	3
74	Surface termination of MgB₂ unveiled by a combination of adsorption experiments and theoretical calculations. Physical Chemistry Chemical Physics, 2019, 21, 7313-7320.	1.3	3
75	Fluorographene: Dichlorocarbene-Functionalized Fluorographene: Synthesis and Reaction Mechanism (Small 31/2015). Small, 2015, 11, 3789-3789.	5.2	2
76	Molecular insights from theoretical calculations explain the differences in affinity and diffusion of airborne contaminants on surfaces of hBN and graphene. Applied Surface Science, 2021, 565, 150382.	3.1	2
77	1D Coordination Ï€â€“d Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles. Angewandte Chemie, 2021, 133, 443-449.	1.6	0