Li-Chun Xu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5332688/publications.pdf

Version: 2024-02-01

57 papers	1,502 citations	331538 21 h-index	315616 38 g-index
57 all docs	57 docs citations	57 times ranked	2227 citing authors

#	Article	IF	Citations
1	Inorganic gas sensing performance of Ï‡3-borophene and the van der Waals heterostructure. Applied Surface Science, 2022, 581, 151906.	3.1	18
2	Enhance the anchoring and catalytic performance of lithium-sulfur batteries for lithium polysulfide by predicted TiS2 monolayer. Materials Today Communications, 2022, 30, 103196.	0.9	6
3	Designing and optimizing Î²1-borophene organic gas sensor: A theoretical study. Surface Science, 2022, 719, 122030.	0.8	8
4	Strain induced magnetic hysteresis in MoS₂ and WS₂ monolayers with symmetric double sulfur vacancy defects. Physical Chemistry Chemical Physics, 2022, 24, 17263-17270.	1.3	1
5	Modelling high performance potassium-ion battery anode materials with two-dimensional vanadium carbide MXene: the role of surface O- and S-terminations. Physical Chemistry Chemical Physics, 2021, 23, 3898-3904.	1.3	12
6	Organic Gas Sensing Performance of the Borophene van der Waals Heterostructure. Journal of Physical Chemistry C, 2021, 125, 427-435.	1.5	30
7	The gas sensing performance of borophene/MoS2 heterostructure. Applied Surface Science, 2020, 504, 144412.	3.1	59
8	Polar, catalytic, and conductive CoSe2/C frameworks for performance enhanced S cathode in Liâ€“S batteries. Journal of Energy Chemistry, 2020, 48, 128-135.	7.1	61
9	A boron-exposed TiB₃ monolayer with a lower electrostatic-potential surface as a higher-performance anode material for Li-ion and Na-ion batteries. Physical Chemistry Chemical Physics, 2020, 22, 22236-22243.	1.3	31
10	Achieving superior high-capacity K-ion batteries with the C57 carbon monolayer anode by first-principles calculations. Applied Surface Science, 2020, 526, 146638.	3.1	12
11	Stable zigzag edges of transition-metal dichalcogenides with high catalytic activity for oxygen reduction. Electrochimica Acta, 2020, 338, 135865.	2.6	14
12	Achieving superior high-capacity batteries with the lightest Ti2C MXene anode by first-principles calculations: Overarching role of S-functionate (Ti 2CS2) and multivalent cations carrier. Journal of Power Sources, 2020, 451, 227791.	4.0	84
13	Sulfur-functionalized vanadium carbide MXene (V₂CS₂) as a promising anchoring material for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2019, 21, 18559-18568.	1.3	96
14	Contrasting Oxygen Reduction Reactions on Zero- and One-Dimensional Defects of MoS₂ for Versatile Applications. ACS Applied Materials & Interfaces, 2019, 11, 46327-46336.	4.0	22
15	Robust negative differential resistance and abnormal magnetoresistance effects in heteroatom-substituted zigzag Î³-graphyne nanoribbon homojunctions. Journal of Materials Chemistry C, 2019, 7, 1359-1369.	2.7	11
16	Insight into the Discharge Products and Mechanism of Room-Temperature Sodiumâ€“Sulfur Batteries: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 3988-3995.	1.5	30
17	Spin-filtering and tunneling magnetoresistance effects in 6,6,12-graphyne-based molecular magnetic tunnel junctions. Physical Chemistry Chemical Physics, 2019, 21, 2734-2742.	1.3	6
18	Chemical optimization towards superior electrocatalysis of Janus 1T-MoSX (Xâ€¯=â€¯O, Se, Te) for hydrogen evolution: Small composition tuning makes big difference. Electrochimica Acta, 2019, 310, 153-161.	2.6	9

#	Article	IF	Citations
19	Rational design of multi-functional CoS@rGO composite for performance enhanced Li-S cathode. Journal of Power Sources, 2019, 421, 132-138.	4.0	54
20	1T-MoS2 monolayer doped with isolated Ni atoms as highly active hydrogen evolution catalysts: A density functional study. Applied Surface Science, 2019, 469, 292-297.	3.1	41
21	Polar and conductive iron carbide@N-doped porous carbon nanosheets as a sulfur host for high performance lithium sulfur batteries. Chemical Engineering Journal, 2019, 358, 962-968.	6.6	91
22	Synthesis of Mesoporous Co₃O₄/NiCo₂O₄ Nanorods and Their Electrochemical Study. Journal of Nanoscience and Nanotechnology, 2019, 19, 47-56.	0.9	15
23	The transport and optoelectronic properties of Î³-graphyne-based molecular magnetic tunnel junctions. Carbon, 2018, 132, 632-640.	5.4	20
24	The intrinsic interface properties of the top and edge 1T/2H MoS2 contact: A first-principles study. Journal of Applied Physics, 2018, 123, .	1.1	19
25	The spin-dependent transport and optoelectronic properties of the 6,6,12-graphyne-based magnetic tunnel junction devices. Organic Electronics, 2018, 53, 1-13.	1.4	5
26	Structural Engineering of Zincâ€Blend/Wurtzite BN Superlattices. ChemistrySelect, 2018, 3, 13641-13646.	0.7	1
27	Modulate the direct-current and alternating-current transport properties of magnetic Î³-graphyne heterojunctions by chemical modification. Journal of Applied Physics, 2018, 124, 084501.	1.1	2
28	Effects of high-k dielectric environment on the full ballistic transport properties of monolayer MoS2 FETs. Journal of Applied Physics, 2017, 121, 144505.	1.1	6
29	The magnetoresistance effect and spin-polarized photocurrent of zigzag graphene-graphyne nanoribbon heterojunctions. Computational Materials Science, 2017, 136, 1-11.	1.4	24
30	Spin-filter effect and spin-polarized optoelectronic properties in annulene-based molecular spintronic devices. Chinese Physics B, 2017, 26, 067201.	0.7	1
31	The tunneling magnetoresistance and spin-polarized optoelectronic properties of graphyne-based molecular magnetic tunnel junctions. Journal Physics D: Applied Physics, 2017, 50, 075103.	1.3	5
32	Cliff-like NiO/Ni3S2 Directly Grown on Ni Foam for Battery-type Electrode with High Area Capacity and Long Cycle Stability. Electrochimica Acta, 2017, 251, 235-243.	2.6	49
33	Effect of edge structure on the activity for hydrogen evolution reaction in MoS2 nanoribbons. Applied Surface Science, 2017, 396, 138-143.	3.1	28
34	Electronic structure and optical absorption properties of -AgVO3 with vacancy defects. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 157101.	0.2	3
35	Bandgap engineering of GaN nanowires. AIP Advances, 2016, 6, .	0.6	13
36	The thermoelectric performance of bulk three-dimensional graphene. Materials Chemistry and Physics, 2016, 183, 6-10.	2.0	15

#	Article	IF	Citations
37	Hydrogenated borophene as a stable two-dimensional Dirac material with an ultrahigh Fermi velocity. Physical Chemistry Chemical Physics, 2016, 18, 27284-27289.	1.3	167
38	The thermal properties and thermoelectric performance ofÎ³-graphyne nanoribbons. Journal Physics D: Applied Physics, 2016, 49, 145102.	1.3	19
39	Design molecular rectifier and photodetector with all-boron fullerene. Solid State Communications, 2015, 217, 38-42.	0.9	30
40	The magnetic and half-metal properties of iron clusters adsorbed on armchair graphene nanoribbon. Computational and Theoretical Chemistry, 2015, 1062, 84-89.	1.1	13
41	Designing electronic anisotropy of three-dimensional carbon allotropes for the all-carbon device. Applied Physics Letters, 2015, 107, 021905.	1.5	2
42	Phosphorene nanoribbons: Passivation effect on bandgap and effective mass. Applied Surface Science, 2015, 324, 640-644.	3.1	30
43	N-F co-doped in titaninum dioxide nanotube of the anatase (101) surface: a first-principles study. Wuli Xuebao/Acta Physica Sinica, 2015, 64, 147103.	0.2	1
44	Magnetic and Quantum Transport Properties of Small-Sized Transition-Metal-Pentalene Sandwich Cluster. Journal of Physical Chemistry C, 2014, 118, 29695-29703.	1.5	7
45	Enhanced visible light photocatalytic activity for the hybrid MoS2/anatase TiO2(0 0 1) nanocomposite: A first-principles study. Chemical Physics Letters, 2014, 612, 285-288.	1.2	27
46	Two dimensional Dirac carbon allotropes from graphene. Nanoscale, 2014, 6, 1113-1118.	2.8	198
47	The adsorption of H 2 on Fe-coated C 5 H 5 and its application in hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 19621-19629.	3.8	5
48	Structural, electronic, and optical absorption properties of TiO2 nanotube adsorbed with Cu n clusters. Science China: Physics, Mechanics and Astronomy, 2014, 57, 1519-1525.	2.0	0
49	Significant interplay effect of silicon dopants on electronic properties in graphene. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1841-1844.	0.9	12
50	Non-collinear magnetic order and spinâ€“orbit coupling effect in 4d transition metal monatomic chains. Journal of Magnetism and Magnetic Materials, 2014, 368, 262-266.	1.0	2
51	Structural and electronic properties of BaCrO4 at high-pressures. Solid State Communications, 2013, 155, 45-48.	0.9	3
52	Why Clorine Is an Inefficient n-Type Dopant in CuInSe2?. Japanese Journal of Applied Physics, 2013, 52, 100208.	0.8	0
53	Wurtzite-type CuInSe2 for high-performance solar cell absorber: ab initio exploration of the new phase structure. Journal of Materials Chemistry, 2012, 22, 21662.	6.7	30
54	Order Structures of Al_xGa_{1â€“x}N Alloys: First-Principles Predictions. Journal of Physical Chemistry C, 2012, 116, 1282-1285.	1.5	12

#	Article	IF	Citations
55	Thermal expansions in wurtzite AlN, GaN, and InN: First-principle phonon calculations. Journal of Applied Physics, 2011, 110, .	1.1	36
56	Theoretical predictions of morphotropic phase boundary in (1â^'x)Na1/2Bi1/2TiO3-xBaTiO3 by first-principle calculations. Applied Physics A: Materials Science and Processing, 2011, 104, 1085-1089.	1.1	5
57	First Principles Study of Dopant Site Selectivity in Ordered Perovskite CaCu 3 Ti 4 O 12. Chinese Physics Letters, 2011, 28, 036107.	1.3	1