# Li-Chun Xu

List of Publications by Year
in descending order

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|---|---|---|---|
| 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 | Two dimensional Dirac carbon allotropes from graphene. Nanoscale, 2014, 6, 1113-1118. | 2.8 | 198 |
| 2 | 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 |
| 3 | Sulfur-functionalized vanadium carbide MXene (V<sub>2</sub>CS<sub>2</sub>) as a promising anchoring material for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2019, 21, 18559-18568. | 1.3 | 96 |
| 4 | 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 |
| 5 | 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 |
| 6 | 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 |
| 7 | The gas sensing performance of borophene/MoS2 heterostructure. Applied Surface Science, 2020, 504, 144412. | 3.1 | 59 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | Thermal expansions in wurtzite AlN, GaN, and InN: First-principle phonon calculations. Journal of Applied Physics, 2011, 110, . | 1.1 | 36 |
| 12 | A boron-exposed TiB<sub>3</sub> 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 |
| 13 | 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 |
| 14 | Design molecular rectifier and photodetector with all-boron fullerene. Solid State Communications, 2015, 217, 38-42. | 0.9 | 30 |
| 15 | Phosphorene nanoribbons: Passivation effect on bandgap and effective mass. Applied Surface Science, 2015, 324, 640-644. | 3.1 | 30 |
| 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 | Organic Gas Sensing Performance of the Borophene van der Waals Heterostructure. Journal of Physical Chemistry C, 2021, 125, 427-435. | 1.5 | 30 |
| 18 | Effect of edge structure on the activity for hydrogen evolution reaction in MoS2 nanoribbons. Applied Surface Science, 2017, 396, 138-143. | 3.1 | 28 |

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|---|---|---|---|
| 19 | 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 |
| 20 | The magnetoresistance effect and spin-polarized photocurrent of zigzag graphene-graphyne nanoribbon heterojunctions. Computational Materials Science, 2017, 136, 1-11. | 1.4 | 24 |
| 21 | Contrasting Oxygen Reduction Reactions on Zero- and One-Dimensional Defects of MoS<sub>2</sub> for Versatile Applications. ACS Applied Materials & Interfaces, 2019, 11, 46327-46336. | 4.0 | 22 |
| 22 | The transport and optoelectronic properties of Î³-graphyne-based molecular magnetic tunnel junctions. Carbon, 2018, 132, 632-640. | 5.4 | 20 |
| 23 | The thermal properties and thermoelectric performance ofÎ³-graphyne nanoribbons. Journal Physics D: Applied Physics, 2016, 49, 145102. | 1.3 | 19 |
| 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 | Inorganic gas sensing performance of Ï‡3-borophene and the van der Waals heterostructure. Applied Surface Science, 2022, 581, 151906. | 3.1 | 18 |
| 26 | The thermoelectric performance of bulk three-dimensional graphene. Materials Chemistry and Physics, 2016, 183, 6-10. | 2.0 | 15 |
| 27 | Synthesis of Mesoporous Co<sub>3</sub>O<sub>4</sub>/NiCo<sub>2</sub>O<sub>4</sub> Nanorods and Their Electrochemical Study. Journal of Nanoscience and Nanotechnology, 2019, 19, 47-56. | 0.9 | 15 |
| 28 | Stable zigzag edges of transition-metal dichalcogenides with high catalytic activity for oxygen reduction. Electrochimica Acta, 2020, 338, 135865. | 2.6 | 14 |
| 29 | 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 |
| 30 | Bandgap engineering of GaN nanowires. AIP Advances, 2016, 6, . | 0.6 | 13 |
| 31 | Order Structures of Al<sub>x</sub>Ga<sub>1â€“x</sub>N Alloys: First-Principles Predictions. Journal of Physical Chemistry C, 2012, 116, 1282-1285. | 1.5 | 12 |
| 32 | 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 |
| 33 | 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 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Designing and optimizing Î²1-borophene organic gas sensor: A theoretical study. Surface Science, 2022, 719, 122030. | 0.8 | 8 |
| 38 | 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 |
| 39 | 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 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | Structural and electronic properties of BaCrO4 at high-pressures. Solid State Communications, 2013, 155, 45-48. | 0.9 | 3 |
| 47 | Electronic structure and optical absorption properties of -AgVO3 with vacancy defects. Wuli Xuebao/Acta Physica Sinica, 2017, 66, 157101. | 0.2 | 3 |
| 48 | 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 |
| 49 | Designing electronic anisotropy of three-dimensional carbon allotropes for the all-carbon device. Applied Physics Letters, 2015, 107, 021905. | 1.5 | 2 |
| 50 | 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 |
| 51 | 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 |
| 52 | Spin-filter effect and spin-polarized optoelectronic properties in annulene-based molecular spintronic devices. Chinese Physics B, 2017, 26, 067201. | 0.7 | 1 |
| 53 | Structural Engineering of Zincâ€Blend/Wurtzite BN Superlattices. ChemistrySelect, 2018, 3, 13641-13646. | 0.7 | 1 |
| 54 | 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 |

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|---|---|---|---|
| 55 | Strain induced magnetic hysteresis in MoS<sub>2</sub> and WS<sub>2</sub> monolayers with symmetric double sulfur vacancy defects. Physical Chemistry Chemical Physics, 2022, 24, 17263-17270. | 1.3 | 1 |
| 56 | Why Clorine Is an Inefficient n-Type Dopant in CuInSe2?. Japanese Journal of Applied Physics, 2013, 52, 100208. | 0.8 | 0 |
| 57 | 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 |