

Qun Yang

List of Publications by Year in descending order

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49
papers

2,099
citations

201674

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times ranked

2217
citing authors

#	ARTICLE	IF	CITATIONS
1	Identification of Interface Structure for a Topological CoS ₂ Single Crystal in Oxygen Evolution Reaction with High Intrinsic Reactivity. ACS Applied Materials & Interfaces, 2022, 14, 19324-19331.	8.0	10
2	Tunable e g Orbital Occupancy in Heusler Compounds for Oxygen Evolution Reaction**. Angewandte Chemie, 2021, 133, 5864-5869.	2.0	12
3	Tunable i e / i g Orbital Occupancy in Heusler Compounds for Oxygen Evolution Reaction**. Angewandte Chemie - International Edition, 2021, 60, 5800-5805.	13.8	45
4	Transition metal on topological chiral semimetal PdGa with tailored hydrogen adsorption and reduction. Npj Computational Materials, 2021, 7, .	8.7	12
5	Topological Engineering of Pt Group Metal Based Chiral Crystals toward High Efficiency Hydrogen Evolution Catalysts. Advanced Materials, 2020, 32, e1908518.	21.0	81
6	In Situ Induction of Strain in Iron Phosphide (FeP ₂) Catalyst for Enhanced Hydroxide Adsorption and Water Oxidation. Advanced Functional Materials, 2020, 30, 1907791.	14.9	55
7	Observation of giant spin-split Fermi-arc with maximal Chern number in the chiral topological semimetal PtGa. Nature Communications, 2020, 11, 2033.	12.8	46
8	Descriptor for Hydrogen Evolution Catalysts Based on the Bulk Band Structure Effect. ACS Catalysis, 2020, 10, 5042-5048.	11.2	46
9	In Situ Modification of a Delafossite-Type PdCoO ₂ Bulk Single Crystal for Reversible Hydrogen Sorption and Fast Hydrogen Evolution. ACS Energy Letters, 2019, 4, 2185-2191.	17.4	34
10	Dirac Nodal Arc Semimetal PtSn ₄ : An Ideal Platform for Understanding Surface Properties and Catalysis for Hydrogen Evolution. Angewandte Chemie - International Edition, 2019, 58, 13107-13112.	13.8	59
11	Dirac Nodal Arc Semimetal PtSn ₄ : An Ideal Platform for Understanding Surface Properties and Catalysis for Hydrogen Evolution. Angewandte Chemie, 2019, 131, 13241-13246.	2.0	28
12	Photothermal effects induced by surface plasmon resonance at graphene/gold nanointerfaces: A multiscale modeling study. Biosensors and Bioelectronics, 2019, 126, 470-477.	10.1	14
13	Intriguing electronic insensitivity and high carrier mobility in monolayer hexagonal YN. Journal of Materials Chemistry C, 2018, 6, 4943-4951.	5.5	28
14	High Selective Gas Detection for small molecules based on Germanium selenide monolayer. Applied Surface Science, 2018, 433, 575-581.	6.1	68
15	Novel GaN-based nanocomposites: Effective band structure and optical property tuning by tensile strain or external field. Applied Surface Science, 2018, 427, 554-562.	6.1	9
16	Interfacial Failure Characterization of Electronic Packaging Component Using a Multiscale Modelling Approach. , 2018, , .		1
17	Adsorption of gas molecules on graphene-like InN monolayer: A first-principle study. Applied Surface Science, 2017, 404, 291-299.	6.1	141
18	Adsorption of gases on monolayer GeSe: A first principle study. , 2017, , .		2

#	ARTICLE	IF	CITATIONS
19	Electrical and optical properties of NO and H ₂ S adsorption on Arsenic Phosphorus. , 2017, , .		0
20	The intriguing electronic and optical properties modulation in blue phosphorene/g-III-nitrides heterostructures. , 2017, , .		0
21	First principle design of CdS/germanene heterostructures with tunable electronic and transport properties. , 2017, , .		0
22	An AlAs/germanene heterostructure with outstanding tunability of electronic properties. , 2017, , .		0
23	Exploration of new ferromagnetic, semiconducting and biocompatible Nb ₃ X ₈ (X = Cl, Br or I) monolayers with considerable visible and infrared light absorption. Nanoscale, 2017, 9, 2992-3001.	5.6	74
24	AlN/BP Heterostructure Photocatalyst for Water Splitting. IEEE Electron Device Letters, 2017, 38, 145-148.	3.9	68
25	The intriguing electronic and optical properties modulation of hydrogen and fluorine codecorated silicene layers. Applied Surface Science, 2017, 398, 73-80.	6.1	12
26	First Principles Investigation of Small Molecules Adsorption on Antimonene. IEEE Electron Device Letters, 2017, 38, 134-137.	3.9	109
27	DFT coupled with NEGF study of ultra-sensitive HCN and HNC gases detection and distinct I _{on} response based on phosphorene. Physical Chemistry Chemical Physics, 2017, 19, 30852-30860.	2.8	26
28	A Novel Ultra-Sensitive Nitrogen Dioxide Sensor Based on Germanium Monosulfide Monolayer. IEEE Electron Device Letters, 2017, 38, 1590-1593.	3.9	21
29	Considering the spin-orbit coupling effect on the photocatalytic performance of AlN/MX ₂ nanocomposites. Journal of Materials Chemistry C, 2017, 5, 9412-9420.	5.5	36
30	Arsenic Phosphorus Monolayer: A Promising Candidate for H ₂ S Sensor and NO Degradation With High Sensitivity and Selectivity. IEEE Electron Device Letters, 2017, 38, 1321-1324.	3.9	23
31	Tunable electronic structure and enhanced optical properties in quasi-metallic hydrogenated/fluorinated SiC heterobilayer. Journal of Materials Chemistry C, 2016, 4, 7406-7414.	5.5	27
32	The electronic and optical properties of silicene/g-ZnS heterobilayers: a theoretical study. Journal of Materials Chemistry C, 2016, 4, 7004-7012.	5.5	34
33	The Influence of Tensile Stress on Polyaniline as Strain Sensor. IEEE Electron Device Letters, 2016, 37, 1636-1638.	3.9	5
34	Two-dimensional GeS with tunable electronic properties via external electric field and strain. Nanotechnology, 2016, 27, 274001.	2.6	85
35	Electronic structure and optical properties of graphene/stanene heterobilayer. Physical Chemistry Chemical Physics, 2016, 18, 16302-16309.	2.8	115
36	First-Principles Study of Sulfur Dioxide Sensor Based on Phosphorenes. IEEE Electron Device Letters, 2016, 37, 660-662.	3.9	110

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37	The electronic and optical properties of novel germanene and antimonene heterostructures. Journal of Materials Chemistry C, 2016, 4, 5434-5441.	5.5	154
38	Tuning the electronic and optical properties of graphane/silicane and fhBN/silicane nanosheets via interfacial dihydrogen bonding and electrical field control. Journal of Materials Chemistry C, 2016, 4, 8962-8972.	5.5	16
39	A first-principle study of H ₂ , CO, CH ₄ , H ₂ S and SO ₂ gas molecules on antimonene. , 2016, , .		1
40	Adsorption of CO ₂ and CO gas on impurity-decorated phosphorenes: A first-principles study. , 2016, , .		1
41	SiGe/h-BN heterostructure with inspired electronic and optical properties: a first-principles study. Journal of Materials Chemistry C, 2016, 4, 10082-10089.	5.5	40
42	An AlAs/germanene heterostructure with tunable electronic and optical properties via external electric field and strain. Journal of Materials Chemistry C, 2016, 4, 8171-8178.	5.5	81
43	Electrical and Optical Properties of Germanene on Single-Layer BeO Substrate. Journal of Physical Chemistry C, 2016, 120, 20350-20356.	3.1	46
44	Design of graphene-like gallium nitride and WS ₂ /WSe ₂ nanocomposites for photocatalyst applications. Science China Materials, 2016, 59, 1027-1036.	6.3	65
45	Theoretical investigation of electric properties of the silicene / fully hydrogenated BN heterobilayer. , 2016, , .		0
46	Enhancement of H ₂ S detection in impurity-doped graphene. , 2016, , .		1
47	Effect of multilayer structure, stacking order and external electric field on the electrical properties of few-layer boron-phosphide. Physical Chemistry Chemical Physics, 2016, 18, 16229-16236.	2.8	68
48	Tuning the electronic properties and work functions of graphane/fully hydrogenated h-BN heterobilayers via heteronuclear dihydrogen bonding and electric field control. Physical Chemistry Chemical Physics, 2016, 18, 16386-16395.	2.8	41
49	Ab Initio Study of the Adsorption of Small Molecules on Stanene. Journal of Physical Chemistry C, 2016, 120, 13987-13994.	3.1	149