

Qun Yang

List of Publications by Year in descending order

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papers

2,099
citations

201674

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50
all docs

50
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50
times ranked

2217
citing authors

#	ARTICLE	IF	CITATIONS
1	The electronic and optical properties of novel germanene and antimonene heterostructures. Journal of Materials Chemistry C, 2016, 4, 5434-5441.	5.5	154
2	Ab Initio Study of the Adsorption of Small Molecules on Stanene. Journal of Physical Chemistry C, 2016, 120, 13987-13994.	3.1	149
3	Adsorption of gas molecules on graphene-like InN monolayer: A first-principle study. Applied Surface Science, 2017, 404, 291-299.	6.1	141
4	Electronic structure and optical properties of graphene/stanene heterobilayer. Physical Chemistry Chemical Physics, 2016, 18, 16302-16309.	2.8	115
5	First-Principles Study of Sulfur Dioxide Sensor Based on Phosphorenes. IEEE Electron Device Letters, 2016, 37, 660-662.	3.9	110
6	First Principles Investigation of Small Molecules Adsorption on Antimonene. IEEE Electron Device Letters, 2017, 38, 134-137.	3.9	109
7	Two-dimensional GeS with tunable electronic properties via external electric field and strain. Nanotechnology, 2016, 27, 274001.	2.6	85
8	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
9	Topological Engineering of Pt-Group-Metal-Based Chiral Crystals toward High-Efficiency Hydrogen Evolution Catalysts. Advanced Materials, 2020, 32, e1908518.	21.0	81
10	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
11	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
12	AlN/BP Heterostructure Photocatalyst for Water Splitting. IEEE Electron Device Letters, 2017, 38, 145-148.	3.9	68
13	High Selective Gas Detection for small molecules based on Germanium selenide monolayer. Applied Surface Science, 2018, 433, 575-581.	6.1	68
14	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
15	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
16	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
17	Electrical and Optical Properties of Germanene on Single-Layer BeO Substrate. Journal of Physical Chemistry C, 2016, 120, 20350-20356.	3.1	46
18	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

#	ARTICLE	IF	CITATIONS
19	Descriptor for Hydrogen Evolution Catalysts Based on the Bulk Band Structure Effect. ACS Catalysis, 2020, 10, 5042-5048.	11.2	46
20	Tunable e_g Orbital Occupancy in Heusler Compounds for Oxygen Evolution Reaction**. Angewandte Chemie - International Edition, 2021, 60, 5800-5805.	13.8	45
21	Tuning the electronic properties and work functions of graphene/fully hydrogenated h-BN heterobilayers via heteronuclear dihydrogen bonding and electric field control. Physical Chemistry Chemical Physics, 2016, 18, 16386-16395.	2.8	41
22	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
23	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
24	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
25	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
26	Intriguing electronic insensitivity and high carrier mobility in monolayer hexagonal YN. Journal of Materials Chemistry C, 2018, 6, 4943-4951.	5.5	28
27	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
28	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
29	DFT coupled with NEGF study of ultra-sensitive HCN and HNC gases detection and distinct $I \propto V$ response based on phosphorene. Physical Chemistry Chemical Physics, 2017, 19, 30852-30860.	2.8	26
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	A Novel Ultra-Sensitive Nitrogen Dioxide Sensor Based on Germanium Monosulfide Monolayer. IEEE Electron Device Letters, 2017, 38, 1590-1593.	3.9	21
32	Tuning the electronic and optical properties of graphene/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
33	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
34	The intriguing electronic and optical properties modulation of hydrogen and fluorine codecorated silicene layers. Applied Surface Science, 2017, 398, 73-80.	6.1	12
35	Tunable e_g Orbital Occupancy in Heusler Compounds for Oxygen Evolution Reaction**. Angewandte Chemie, 2021, 133, 5864-5869.	2.0	12
36	Transition metal on topological chiral semimetal PdGa with tailored hydrogen adsorption and reduction. Npj Computational Materials, 2021, 7, .	8.7	12

#	ARTICLE	IF	CITATIONS
37	Identification of Interface Structure for a Topological CoS_2 Single Crystal in Oxygen Evolution Reaction with High Intrinsic Reactivity. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 19324-19331.	8.0	10
38	Novel GaN-based nanocomposites: Effective band structure and optical property tuning by tensile strain or external field. <i>Applied Surface Science</i> , 2018, 427, 554-562.	6.1	9
39	The Influence of Tensile Stress on Polyaniline as Strain Sensor. <i>IEEE Electron Device Letters</i> , 2016, 37, 1636-1638.	3.9	5
40	Adsorption of gases on monolayer GeSe: A first principle study. , 2017, , .		2
41	A first-principle study of H_2 , CO, CH_4 , H_2S and SO_2 gas molecules on antimonene. , 2016, , .		1
42	Adsorption of CO_2 and CO gas on impurity-decorated phosphorenes: A first-principles study. , 2016, , .		1
43	Enhancement of H_2S detection in impurity-doped graphene. , 2016, , .		1
44	Interfacial Failure Characterization of Electronic Packaging Component Using a Multiscale Modelling Approach. , 2018, , .		1
45	Theoretical investigation of electric properties of the silicene / fully hydrogenated BN heterobilayer. , 2016, , .		0
46	Electrical and optical properties of NO and H_2S adsorption on Arsenic Phosphorus. , 2017, , .		0
47	The intriguing electronic and optical properties modulation in blue phosphorene/g-III-nitrides heterostructures. , 2017, , .		0
48	First principle design of CdS/germanene heterostructures with tunable electronic and transport properties. , 2017, , .		0
49	An AlAs/germanene heterostructure with outstanding tunability of electronic properties. , 2017, , .		0