Jyh-Pin Chou

List of Publications by Year
in descending order

72	3,316	159358 30	149479 56
papers	citations	h-index	g-index

73	73	73	3127
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures. Physical Chemistry Chemical Physics, 2017, 19, 17324-17330.	1.3	180
2	Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. Applied Physics Letters, 2017, 110, .	1.5	166
3	Color Centers in Hexagonal Boron Nitride Monolayers: A Group Theory and Ab Initio Analysis. ACS Photonics, 2018, 5, 1967-1976.	3.2	157
4	Electronic and magnetic properties of 4d series transition metal substituted graphene: A first-principles study. Carbon, 2017, 120, 265-273.	5.4	135
5	Effects of structural imperfection on the electronic properties of graphene/WSe₂ heterostructures. Journal of Materials Chemistry C, 2017, 5, 10383-10390.	2.7	131
6	Proper Surface Termination for Luminescent Near-Surface NV Centers in Diamond. Nano Letters, 2014, 14, 4772-4777.	4.5	125
7	Ab initio theory of the negatively charged boron vacancy qubit in hexagonal boron nitride. Npj Computational Materials, 2020, 6, .	3.5	118
8	Platinum-trimer decorated cobalt-palladium core-shell nanocatalyst with promising performance for oxygen reduction reaction. Nature Communications, 2019, 10, 440.	5.8	115
9	First-Principles Study on Transition-Metal Dichalcogenide/BSe van der Waals Heterostructures: A Promising Water-Splitting Photocatalyst. Journal of Physical Chemistry C, 2019, 123, 22742-22751.	1.5	110
10	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (Xâ€‰â€‰=â€‰â€‰Ga, Al) van der Waals heterostructure. Journal Physics D: Applied Physics, 2020, 53, 185504.	1.3	110
11	Exceptional Optical Absorption of Buckled Arsenene Covering a Broad Spectral Range by Molecular Doping. ACS Omega, 2018, 3, 8514-8520.	1.6	107
12	Transition-metal dichalcogenides/Mg(OH)₂ van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 1791-1796.	1.3	106
13	Material platforms for defect qubits and single-photon emitters. Applied Physics Reviews, 2020, 7, .	5.5	96
14	Achieving large uniform tensile elasticity in microfabricated diamond. Science, 2021, 371, 76-78.	6.0	95
15	Few-Layer PdSe₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. ACS Omega, 2018, 3, 5971-5979.	1.6	87
16	Point Defects in Blue Phosphorene. Chemistry of Materials, 2019, 31, 8129-8135.	3.2	86
17	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. Applied Surface Science, 2018, 427, 609-612.	3.1	79
18	A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. ACS Omega, 2019, 4, 21689-21697.	1.6	78

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19	First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures. Physical Chemistry Chemical Physics, 2018, 20, 24726-24734.	1.3	77
20	Evidence for Primal sp² Defects at the Diamond Surface: Candidates for Electron Trapping and Noise Sources. Advanced Materials Interfaces, 2019, 6, 1801449.	1.9	75
21	A Strategy to Create Spin-Split Metallic Bands on Silicon Using a Dense Alloy Layer. Scientific Reports, 2014, 4, 4742.	1.6	65
22	Nitrogen-Terminated Diamond (111) Surface for Room-Temperature Quantum Sensing and Simulation. Nano Letters, 2017, 17, 2294-2298.	4.5	65
23	Nitrogen Terminated Diamond. Advanced Materials Interfaces, 2015, 2, 1500079.	1.9	61
24	A MoSSe/blue phosphorene vdw heterostructure with energy conversion efficiency of 19.9% for photocatalytic water splitting. Semiconductor Science and Technology, 2020, 35, 125008.	1.0	56
25	Tunable Schottky barrier in graphene/graphene-like germanium carbide van der Waals heterostructure. Scientific Reports, 2019, 9, 5208.	1.6	48
26	Ab initiorandom structure search for 13-atom clusters of fcc elements. Journal of Physics Condensed Matter, 2013, 25, 125305.	0.7	45
27	13-atom metallic clusters studied by density functional theory: Dependence on exchange-correlation approximations and pseudopotentials. Physical Review B, 2009, 80, .	1.1	42
28	Weak Câ€“Hâ‹¯Fâ€“C hydrogen bonds make a big difference in graphane/fluorographane and fluorographene/fluorographane bilayers. Physical Chemistry Chemical Physics, 2017, 19, 28127-28132.	1.3	41
29	Van der Waals interaction in a boron nitride bilayer. New Journal of Physics, 2014, 16, 113015.	1.2	37
30	Phase transformation assisted twinning in a face-centered-cubic FeCrNiCoAl high entropy alloy. Acta Materialia, 2019, 181, 491-500.	3.8	37
31	Stepwise self-assembly of C60 mediated by atomic scale moirÃ© magnifiers. Nature Communications, 2013, 4, 1679.	5.8	31
32	Unravelling the Role of Structural Geometry and Chemical State of Well-Defined Oxygen Vacancies on Pristine CeO₂ for H₂O₂ Activation. Journal of Physical Chemistry Letters, 2020, 11, 5390-5396.	2.1	30
33	Promotion of CO Oxidation on Bimetallic Auâ^'Ag(110) Surfaces: A Combined Microscopic and Theoretical Study. Journal of Physical Chemistry C, 2009, 113, 13151-13159.	1.5	28
34	Programming ORR Activity of Ni/NiO_x@Pd Electrocatalysts via Controlling Depth of Surface-Decorated Atomic Pt Clusters. ACS Omega, 2018, 3, 8733-8744.	1.6	27
35	Pt₃ clusters-decorated Co@Pd and Ni@Pd model coreâ€“shell catalyst design for the oxygen reduction reaction: a DFT study. Journal of Materials Chemistry A, 2018, 6, 23326-23335.	5.2	26
36	Nitrogen-vacancy diamond sensor: novel diamond surfaces from ab initio simulations. MRS Communications, 2017, 7, 551-562.	0.8	25

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37	Giant shift upon strain on the fluorescence spectrum of VNNB color centers in h-BN. Npj Quantum Information, 2020, 6, .	2.8	25
38	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. Carbon, 2019, 145, 273-280.	5.4	24
39	Two-Dimensional Inâ€“Sb Compound on Silicon as a Quantum Spin Hall Insulator. Nano Letters, 2018, 18, 4338-4345.	4.5	23
40	Photocatalytic activity enhancement of Cu₂O cubes functionalized with 2-ethynyl-6-methoxynaphthalene through band structure modulation. Journal of Materials Chemistry C, 2022, 10, 3980-3989.	2.7	22
41	Synthesis of two-dimensional TlxBi1â^'x compounds and Archimedean encoding of their atomic structure. Scientific Reports, 2016, 6, 19446.	1.6	21
42	Heterogeneous Cuâ€“Pd binary interface boosts stability and mass activity of atomic Pt clusters in the oxygen reduction reaction. Nanoscale, 2017, 9, 7207-7216.	2.8	21
43	Interfacial atomic Ni tetragon intercalation in a NiO₂-to-Pd hetero-structure triggers superior HER activity to the Pt catalyst. Journal of Materials Chemistry A, 2021, 9, 12019-12028.	5.2	19
44	Atomic structure and electronic properties of the In/Si(111)2<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>Ã—</mml:mo></mml:math>2 surface. Physical Review B, 2014, 89, .	1.1	18
45	First-Principles Study of Charge Diffusion between Proximate Solid-State Qubits and Its Implications on Sensor Applications. Physical Review Letters, 2018, 120, 136401.	2.9	16
46	The influence of dilute aluminum and molybdenum on stacking fault and twin formation in FeNiCoCr-based high entropy alloys based on density functional theory. Scientific Reports, 2019, 9, 10940.	1.6	16
47	Nanoisozymes: The Origin behind Pristine CeO₂ as Enzyme Mimetics. Chemistry - A European Journal, 2020, 26, 10598-10606.	1.7	16
48	Collaboration between a Pt-dimer and neighboring Coâ€“Pd atoms triggers efficient pathways for oxygen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 1822-1834.	1.3	16
49	Molecular doping of blue phosphorene: a first-principles investigation. Journal of Physics Condensed Matter, 2020, 32, 055501.	0.7	14
50	Atomic scale Pt decoration promises oxygen reduction properties of Co@Pd nanocatalysts in alkaline electrolytes for 310k redox cycles. Sustainable Energy and Fuels, 2018, 2, 946-957.	2.5	13
51	Trimeric precursors in formation of Al magic clusters on a Si(111)-<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>7</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>7</mml:mn></mml:mrow></mml:math>su Physical Review B, 2011, 83, .	1.1	12
52	Peculiar diffusion of C60 on In-adsorbed Si(111)âˆš3 Ã— âˆš3-Au surface. Surface Science, 2013, 616, 44-50.	0.8	12
53	New structural model for Na6Si3 surface magic cluster on the Si(111)-7Ã—7 surface. Surface Science, 2013, 616, 137-142.	0.8	11
54	All-optical hyperpolarization of electron and nuclear spins in diamond. Physical Review B, 2017, 96, .	1.1	11

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55	One-dimensional Rashba states in Pb atomic chains on a semiconductor surface. Physical Review B, 2020, 102, .	1.1	11
56	4-Nitrophenylacetylene-modified Cu₂O cubes and rhombic dodecahedra showing superior photocatalytic activity through surface band structure modulation. Journal of Materials Chemistry C, 2022, 10, 8422-8431.	2.7	11
57	Adsorption and diffusion of an Au atom and dimer on a Î¸-Al2O3 (001) surface. Surface Science, 2011, 605, 1122-1128.	0.8	10
58	Dim C60 fullerenes on Si(111) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si7.gif" overflow="scroll"><mml:mrow><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>Ã—</mml:mo><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mi mathvariant="normal">Ag</mml:mi></mml:mrow></mml:math> surface. Surface Science, 2013, 612, 31-36.	0.8	10
59	A study of strain-induced indirect-direct bandgap transition for silicon nanowire applications. Journal of Applied Physics, 2019, 125, .	1.1	10
60	Double-atomic layer of Tl on Si(111): Atomic arrangement and electronic properties. Surface Science, 2018, 668, 17-22.	0.8	9
61	Catalyzed Decomposition of Methanol-d₄ on Vanadium Nanoclusters Supported on an Ultrathin Film of Al₂O₃/NiAl(100). Journal of Physical Chemistry C, 2022, 126, 3903-3914.	1.5	9
62	Interplay between adsorbed C60 fullerenes and point defects on a Si(111)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si8.gif" overflow="scroll"><mml:mrow><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt><mml:mo>Ã—</mml:mo><mml:msqrt><mml:mn>3</mml:mn></mml:msqrt></mml:mrow></mml:math> reconstructed surface. Surface Science, 2011, 605, 2050-2054.	0.8	6
63	â€œDeep Ultra-Strengthâ€•Induced Band Structure Evolution in Silicon Nanowires. Journal of Physical Chemistry C, 2018, 122, 15780-15785.	1.5	5
64	Cyclability evaluation on Si based Negative Electrode in Lithium ion Battery by Graphite Phase Evolution: an operando X-ray diffraction study. Scientific Reports, 2019, 9, 1299.	1.6	5
65	Tri-atomic Pt clusters induce effective pathways in a Co_{core}â€“Pd_{shell} nanocatalyst surface for a high-performance oxygen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 18012-18025.	1.3	5
66	Solar Photoelectroreduction of Nitrate Ions on PbI 2 /CuI Nanocomposite Electrodes. Solar Rrl, 2021, 5, 2000418.	3.1	4
67	Accurate and Efficient Quantum Computations of Molecular Properties Using Daubechies Wavelet Molecular Orbitals: A Benchmark Study against Experimental Data. PRX Quantum, 2022, 3, .	3.5	4
68	Broken Even-Odd Symmetry in Self-Selection of Distances between Nanoclusters due to the Presence or Absence of Topological Solitons. Physical Review Letters, 2011, 106, 166101.	2.9	3
69	2D Tlâ€“Pb compounds on Ge(1â€‰1â€‰1) surface: atomic arrangement and electronic band structure. Journal of Physics Condensed Matter, 2017, 29, 035001.	0.7	3
70	Cooperative phenomena in self-assembled nucleation of 3Ã—4-In/Si(100) surface magic clusters. Surface Science, 2010, 604, 1116-1120.	0.8	2
71	An optimized random structures generator governed by chemical short-range order for multi-component solid solutions. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 085007.	0.8	2
72	Phase Transformation Assisted Twinning in Face-Centered-Cubic FeCrNiCoAl _{0.36}. SSRN Electronic Journal, 0, , .	0.4	0