

Jyh-Pin Chou

List of Publications by Year in descending order

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72
papers

3,316
citations

159358

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149479

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73
all docs

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docs citations

73
times ranked

3127
citing authors

#	ARTICLE	IF	CITATIONS
1	Photocatalytic activity enhancement of Cu ₂ O cubes functionalized with 2-ethynyl-6-methoxynaphthalene through band structure modulation. Journal of Materials Chemistry C, 2022, 10, 3980-3989.	2.7	22
2	Catalyzed Decomposition of Methanol-d ₄ on Vanadium Nanoclusters Supported on an Ultrathin Film of Al ₂ O ₃ /NiAl(100). Journal of Physical Chemistry C, 2022, 126, 3903-3914.	1.5	9
3	4-Nitrophenylacetylene-modified Cu ₂ O 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
4	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
5	Collaboration between a Pt-dimer and neighboring Co-Pd atoms triggers efficient pathways for oxygen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 1822-1834.	1.3	16
6	Solar Photoelectroreduction of Nitrate Ions on Pbl ₂ /CuI Nanocomposite Electrodes. Solar Rrl, 2021, 5, 2000418.	3.1	4
7	Tri-atomic Pt clusters induce effective pathways in a Co _{core} -Pd _{shell} nanocatalyst surface for a high-performance oxygen reduction reaction. Physical Chemistry Chemical Physics, 2021, 23, 18012-18025.	1.3	5
8	Achieving large uniform tensile elasticity in microfabricated diamond. Science, 2021, 371, 76-78.	6.0	95
9	Interfacial atomic Ni tetragon intercalation in a NiO ₂ -to-Pd hetero-structure triggers superior HER activity to the Pt catalyst. Journal of Materials Chemistry A, 2021, 9, 12019-12028.	5.2	19
10	Molecular doping of blue phosphorene: a first-principles investigation. Journal of Physics Condensed Matter, 2020, 32, 055501.	0.7	14
11	Giant shift upon strain on the fluorescence spectrum of VNNB color centers in h-BN. Npj Quantum Information, 2020, 6, .	2.8	25
12	Material platforms for defect qubits and single-photon emitters. Applied Physics Reviews, 2020, 7, .	5.5	96
13	One-dimensional Rashba states in Pb atomic chains on a semiconductor surface. Physical Review B, 2020, 102, .	1.1	11
14	Ab initio theory of the negatively charged boron vacancy qubit in hexagonal boron nitride. Npj Computational Materials, 2020, 6, .	3.5	118
15	Unravelling the Role of Structural Geometry and Chemical State of Well-Defined Oxygen Vacancies on Pristine CeO ₂ for H ₂ O ₂ Activation. Journal of Physical Chemistry Letters, 2020, 11, 5390-5396.	2.1	30
16	Nanoisozymes: The Origin behind Pristine CeO ₂ as Enzyme Mimetics. Chemistry - A European Journal, 2020, 26, 10598-10606.	1.7	16
17	High-efficiency photocatalyst for water splitting: a Janus MoSSe/XN (X=Ga, Al) van der Waals heterostructure. Journal Physics D: Applied Physics, 2020, 53, 185504.	1.3	110
18	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

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19	The influence of dilute aluminum and molybdenum on stacking fault and twin formation in FeNiCoCr-based high entropy alloys based on density functional theory. <i>Scientific Reports</i> , 2019, 9, 10940.	1.6	16
20	Phase transformation assisted twinning in a face-centered-cubic FeCrNiCoAl high entropy alloy. <i>Acta Materialia</i> , 2019, 181, 491-500.	3.8	37
21	Tunable Schottky barrier in graphene/graphene-like germanium carbide van der Waals heterostructure. <i>Scientific Reports</i> , 2019, 9, 5208.	1.6	48
22	A study of strain-induced indirect-direct bandgap transition for silicon nanowire applications. <i>Journal of Applied Physics</i> , 2019, 125, .	1.1	10
23	First-Principles Study on Transition-Metal Dichalcogenide/BSe van der Waals Heterostructures: A Promising Water-Splitting Photocatalyst. <i>Journal of Physical Chemistry C</i> , 2019, 123, 22742-22751.	1.5	110
24	Point Defects in Blue Phosphorene. <i>Chemistry of Materials</i> , 2019, 31, 8129-8135.	3.2	86
25	Oxygenated (113) diamond surface for nitrogen-vacancy quantum sensors with preferential alignment and long coherence time from first principles. <i>Carbon</i> , 2019, 145, 273-280.	5.4	24
26	Platinum-trimer decorated cobalt-palladium core-shell nanocatalyst with promising performance for oxygen reduction reaction. <i>Nature Communications</i> , 2019, 10, 440.	5.8	115
27	Transition-metal dichalcogenides/Mg(OH) ₂ van der Waals heterostructures as promising water-splitting photocatalysts: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1791-1796.	1.3	106
28	Cyclability evaluation on Si based Negative Electrode in Lithium ion Battery by Graphite Phase Evolution: an operando X-ray diffraction study. <i>Scientific Reports</i> , 2019, 9, 1299.	1.6	5
29	An optimized random structures generator governed by chemical short-range order for multi-component solid solutions. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019, 27, 085007.	0.8	2
30	A van der Waals Heterostructure Based on Graphene-like Gallium Nitride and Boron Selenide: A High-Efficiency Photocatalyst for Water Splitting. <i>ACS Omega</i> , 2019, 4, 21689-21697.	1.6	78
31	Evidence for Primal sp ² Defects at the Diamond Surface: Candidates for Electron Trapping and Noise Sources. <i>Advanced Materials Interfaces</i> , 2019, 6, 1801449.	1.9	75
32	Color Centers in Hexagonal Boron Nitride Monolayers: A Group Theory and Ab Initio Analysis. <i>ACS Photonics</i> , 2018, 5, 1967-1976.	3.2	157
33	Atomic scale Pt decoration promises oxygen reduction properties of Co@Pd nanocatalysts in alkaline electrolytes for 310k redox cycles. <i>Sustainable Energy and Fuels</i> , 2018, 2, 946-957.	2.5	13
34	First-Principles Study of Charge Diffusion between Proximate Solid-State Qubits and Its Implications on Sensor Applications. <i>Physical Review Letters</i> , 2018, 120, 136401.	2.9	16
35	Double-atomic layer of Tl on Si(111): Atomic arrangement and electronic properties. <i>Surface Science</i> , 2018, 668, 17-22.	0.8	9
36	Magnetism in non-metal atoms adsorbed graphene-like gallium nitride monolayers. <i>Applied Surface Science</i> , 2018, 427, 609-612.	3.1	79

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37	First-principles calculations of the electronic properties of SiC-based bilayer and trilayer heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 24726-24734.	1.3	77
38	Pt ₃ clusters-decorated Co@Pd and Ni@Pd model core-shell catalyst design for the oxygen reduction reaction: a DFT study. <i>Journal of Materials Chemistry A</i> , 2018, 6, 23326-23335.	5.2	26
39	Deep Ultra-Strength-Induced Band Structure Evolution in Silicon Nanowires. <i>Journal of Physical Chemistry C</i> , 2018, 122, 15780-15785.	1.5	5
40	Exceptional Optical Absorption of Buckled Arsenene Covering a Broad Spectral Range by Molecular Doping. <i>ACS Omega</i> , 2018, 3, 8514-8520.	1.6	107
41	Programming ORR Activity of Ni/NiO _x @Pd Electrocatalysts via Controlling Depth of Surface-Decorated Atomic Pt Clusters. <i>ACS Omega</i> , 2018, 3, 8733-8744.	1.6	27
42	Few-Layer PdSe ₂ Sheets: Promising Thermoelectric Materials Driven by High Valley Convergence. <i>ACS Omega</i> , 2018, 3, 5971-5979.	1.6	87
43	Two-Dimensional InSb Compound on Silicon as a Quantum Spin Hall Insulator. <i>Nano Letters</i> , 2018, 18, 4338-4345.	4.5	23
44	Heterogeneous CuPd binary interface boosts stability and mass activity of atomic Pt clusters in the oxygen reduction reaction. <i>Nanoscale</i> , 2017, 9, 7207-7216.	2.8	21
45	Tunable Schottky barrier in van der Waals heterostructures of graphene and g-GaN. <i>Applied Physics Letters</i> , 2017, 110, .	1.5	166
46	Electronic and magnetic properties of 4d series transition metal substituted graphene: A first-principles study. <i>Carbon</i> , 2017, 120, 265-273.	5.4	135
47	2D TlPb compounds on Ge(111) surface: atomic arrangement and electronic band structure. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 035001.	0.7	3
48	Electronic properties of blue phosphorene/graphene and blue phosphorene/graphene-like gallium nitride heterostructures. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17324-17330.	1.3	180
49	Nitrogen-Terminated Diamond (111) Surface for Room-Temperature Quantum Sensing and Simulation. <i>Nano Letters</i> , 2017, 17, 2294-2298.	4.5	65
50	Effects of structural imperfection on the electronic properties of graphene/WSe ₂ heterostructures. <i>Journal of Materials Chemistry C</i> , 2017, 5, 10383-10390.	2.7	131
51	Weak C-H...F hydrogen bonds make a big difference in graphene/fluorographane and fluorographane/fluorographane bilayers. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 28127-28132.	1.3	41
52	Nitrogen-vacancy diamond sensor: novel diamond surfaces from ab initio simulations. <i>MRS Communications</i> , 2017, 7, 551-562.	0.8	25
53	All-optical hyperpolarization of electron and nuclear spins in diamond. <i>Physical Review B</i> , 2017, 96, .	1.1	11
54	Synthesis of two-dimensional TlxBi _{1-x} compounds and Archimedean encoding of their atomic structure. <i>Scientific Reports</i> , 2016, 6, 19446.	1.6	21

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55	Nitrogen Terminated Diamond. <i>Advanced Materials Interfaces</i> , 2015, 2, 1500079.	1.9	61
56	Atomic structure and electronic properties of the $\text{In}/\text{Si}(111)2 \times 2$ surface. <i>Physical Review B</i> , 2014, 89, .	1.1	18
57	Van der Waals interaction in a boron nitride bilayer. <i>New Journal of Physics</i> , 2014, 16, 113015.	1.2	37
58	Proper Surface Termination for Luminescent Near-Surface NV Centers in Diamond. <i>Nano Letters</i> , 2014, 14, 4772-4777.	4.5	125
59	A Strategy to Create Spin-Split Metallic Bands on Silicon Using a Dense Alloy Layer. <i>Scientific Reports</i> , 2014, 4, 4742.	1.6	65
60	Stepwise self-assembly of C60 mediated by atomic scale moiré magnifiers. <i>Nature Communications</i> , 2013, 4, 1679.	5.8	31
61	Dim C60 fullerenes on $\text{Si}(111) \sqrt{3} \times \sqrt{3}$ surface. <i>Surface Science</i> , 2013, 612, 31-36.	0.8	6
62	Peculiar diffusion of C60 on In-adsorbed $\text{Si}(111) \sqrt{3} \times \sqrt{3}$ -Au surface. <i>Surface Science</i> , 2013, 616, 44-50.	0.8	12
63	New structural model for Na_6Si_3 surface magic cluster on the $\text{Si}(111) \sqrt{7} \times \sqrt{7}$ surface. <i>Surface Science</i> , 2013, 616, 137-142.	0.8	11
64	Ab initio random structure search for 13-atom clusters of fcc elements. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 125305.	0.7	45
65	Interplay between adsorbed C60 fullerenes and point defects on a $\text{Si}(111) \sqrt{3} \times \sqrt{3}$ reconstructed surface. <i>Surface Science</i> , 2011, 605, 2050-2054.	0.8	6
66	Adsorption and diffusion of an Au atom and dimer on a $\text{Al}_2\text{O}_3(001)$ surface. <i>Surface Science</i> , 2011, 605, 1122-1128.	0.8	10
67	Trimeric precursors in formation of Al magic clusters on a $\text{Si}(111) \sqrt{7} \times \sqrt{7}$ surface. <i>Physical Review B</i> , 2011, 83, .	1.1	12
68	Broken Even-Odd Symmetry in Self-Selection of Distances between Nanoclusters due to the Presence or Absence of Topological Solitons. <i>Physical Review Letters</i> , 2011, 106, 166101.	2.9	3
69	Cooperative phenomena in self-assembled nucleation of 3×3 - $\text{In}/\text{Si}(100)$ surface magic clusters. <i>Surface Science</i> , 2010, 604, 1116-1120.	0.8	2
70	13-atom metallic clusters studied by density functional theory: Dependence on exchange-correlation approximations and pseudopotentials. <i>Physical Review B</i> , 2009, 80, .	1.1	42
71	Promotion of CO Oxidation on Bimetallic $\text{Au}^{\sim}\text{Ag}(110)$ Surfaces: A Combined Microscopic and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 13151-13159.	1.5	28
72	Phase Transformation Assisted Twinning in Face-Centered-Cubic $\text{FeCrNiCoAl}_{0.36}$. <i>SSRN Electronic Journal</i> , 0, .	0.4	0