

Hong-Kuan Yuan

List of Publications by Year in descending order

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papers

1,745
citations

236833

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all docs

78
docs citations

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times ranked

1552
citing authors

#	ARTICLE	IF	CITATIONS
1	Interfacial Defect Passivation and Stress Release via Multi-Active-Site Ligand Anchoring Enables Efficient and Stable Methylammonium-Free Perovskite Solar Cells. ACS Energy Letters, 2021, 6, 2526-2538.	8.8	170
2	A two-dimensional layered CdS/C ₂ N heterostructure for visible-light-driven photocatalysis. Physical Chemistry Chemical Physics, 2017, 19, 28216-28224.	1.3	75
3	A hybrid density functional study on the visible light photocatalytic activity of (Mo,Cr)-N codoped KNbO ₃ . Physical Chemistry Chemical Physics, 2015, 17, 28743-28753.	1.3	67
4	Spin-gapless semiconductors for future spintronics and electronics. Physics Reports, 2020, 888, 1-57.	10.3	64
5	Two dimensional InSe/C ₂ N van der Waals heterojunction as enhanced visible-light-responsive photocatalyst for water splitting. Applied Surface Science, 2019, 485, 375-380.	3.1	61
6	Direct Z-scheme photocatalytic overall water splitting on two dimensional MoSe ₂ /SnS ₂ heterojunction. International Journal of Hydrogen Energy, 2020, 45, 2785-2793.	3.8	54
7	Density-functional study of Sc _n (n=2-16) clusters: Lowest-energy structures, electronic structure, and magnetism. Physical Review B, 2006, 74, .	1.1	51
8	Monolayer $Ce_{1-x}Mg_x$: An intrinsic room-temperature ferrovalley semiconductor. Physical Review B, 2022, 105, .	1.4	50
9	Density-functional calculations of the structure and electronic and magnetic properties of small yttrium clusters Y _n (n=2-17). Physical Review B, 2007, 75, .	1.1	44
10	The spin and orbital moment of Fe _n (n = 2-20) clusters. Journal of Chemical Physics, 2013, 139, 034314.	1.2	42
11	L ₂₁ and XA ordering competition in titanium-based full-Heusler alloys. Journal of Materials Chemistry C, 2017, 5, 11559-11564.	2.7	42
12	BiOX/BiOY (X, Y = F, Cl, Br, I) superlattices for visible light photocatalysis applications. RSC Advances, 2016, 6, 91508-91516.	1.7	41
13	A two-dimensional h-BN/C ₂ N heterostructure as a promising metal-free photocatalyst for overall water-splitting. Physical Chemistry Chemical Physics, 2020, 22, 24446-24454.	1.3	41
14	Site preference and tetragonal distortion in palladium-rich Heusler alloys. IUCr, 2019, 6, 218-225.	1.0	41
15	High-capacity hydrogen storage in Li-decorated (AlN) _n (n=12, 24, 36) nanocages. International Journal of Hydrogen Energy, 2014, 39, 3780-3789.	3.8	39
16	Thermoelectric Performance of Two-Dimensional AlX (X = S, Se, Te): A First-Principles-Based Transport Study. ACS Omega, 2019, 4, 17773-17781.	1.6	38
17	ZnO/MoX ₂ (X = S, Se) composites used for visible light photocatalysis. RSC Advances, 2018, 8, 10828-10835.	1.7	36
18	Bandgap engineering and charge separation in two-dimensional GaS-based van der Waals heterostructures for photocatalytic water splitting. Applied Surface Science, 2018, 439, 374-379.	3.1	36

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19	Strain-engineered topological phase transitions in ferrovalley HfTe_2 monolayer. <i>Physical Review B</i> , 2022, 105, .		
20	Bandgap Engineering of the g-ZnO Nanosheet via Cationic/Anionic Passivated Codoping for Visible-Light-Driven Photocatalysis. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18534-18543.	1.5	33
21	Structural and Magnetic Properties of Small 4d Transition Metal Clusters: Role of Spin-Orbit Coupling. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11673-11684.	1.1	31
22	Band gap engineering of SnS_2 nanosheets by anionic/anion codoping for visible-light photocatalysis. <i>RSC Advances</i> , 2018, 8, 3304-3311.	1.7	31
23	Structural, electronic, elastic, and thermodynamic properties of the spin-gapless semiconducting Mn_2CoAl inverse Heusler alloy under pressure. <i>Physica Status Solidi (B): Basic Research</i> , 2015, 252, 2830-2839.	0.7	30
24	Double-Hole-Mediated Codoping on KNbO_3 for Visible Light Photocatalysis. <i>Inorganic Chemistry</i> , 2016, 55, 9620-9631.	1.9	30
25	Spin-orbit effect and magnetic anisotropy in Pt clusters. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 331, 7-16.	1.0	27
26	The mixing effect of organic cations on the structural, electronic and optical properties of $\text{FA}_{1-x}\text{MA}_x\text{PbI}_3$ perovskites. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 941-950.	1.3	24
27	Bilayer $\text{MoTe}_2/\text{XS}_2$ ($X = \text{Hf, Sn, Zr}$) heterostructures with efficient carrier separation and light absorption for photocatalytic water splitting into hydrogen. <i>Applied Surface Science</i> , 2021, 544, 148842.	3.1	24
28	Structural and magnetic properties of CoPt clusters. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2014, 378, 198-206.	0.9	23
29	Monolayer gadolinium halides, GdX_2 ($X = \text{F, Cl, Br}$): intrinsic ferrovalley materials with spontaneous spin and valley polarizations. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3865-3874.	1.3	23
30	Strain-tunable electronic and optical properties in two dimensional $\text{GaSe/g-C}_3\text{N}_4$ van der Waals heterojunction as photocatalyst for water splitting. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 118, 113896.	1.3	22
31	Efficient charge separation and visible-light response in bilayer HfS_2 -based van der Waals heterostructures. <i>RSC Advances</i> , 2018, 8, 18889-18895.	1.7	20
32	Electronic and optical properties of perovskite compounds $\text{MA}_{1-x}\text{FA}_x\text{PbI}_3$ ($X = \text{Cl, Br}$) explored for photovoltaic applications. <i>RSC Advances</i> , 2019, 9, 7015-7024.	1.7	20
33	Bilayer $\text{MoSe}_2/\text{HfS}_2$ Nanocomposite as a Potential Visible-Light-Driven Z-Scheme Photocatalyst. <i>Nanomaterials</i> , 2019, 9, 1706.	1.9	20
34	Two-dimensional hexagonal manganese carbide monolayer with intrinsic ferromagnetism and half-metallicity. <i>New Journal of Physics</i> , 2020, 22, 103049.	1.2	19
35	Geometrical structure and spin order of Gd_{13} cluster. <i>Journal of Chemical Physics</i> , 2011, 135, 114512.	1.2	18
36	Mechanism for hydrogen evolution from water splitting based on a $\text{MoS}_2/\text{WSe}_2$ heterojunction photocatalyst: a first-principle study. <i>RSC Advances</i> , 2020, 10, 41127-41136.	1.7	18

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37	Hourglass Weyl and Dirac nodal line phonons, and drumhead-like and torus phonon surface states in orthorhombic-type KCuS. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2752-2757.	1.3	18
38	Two-dimensional CdS/SnS ₂ heterostructure: a highly efficient direct Z-scheme water splitting photocatalyst. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3826-3833.	1.3	18
39	Robust spin manipulation in 2D organometallic Kagome lattices: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 11045-11052.	1.3	17
40	Two dimensional CdS/ZnO type-II heterostructure used for photocatalytic water-splitting. <i>Nanotechnology</i> , 2020, 31, 485701.	1.3	15
41	Intrinsic ferromagnetism in 2D h-CrC semiconductors with strong magnetic anisotropy and high Curie temperatures. <i>Journal of Materials Chemistry C</i> , 2021, 9, 16495-16505.	2.7	15
42	Theoretical insight into two-dimensional g-C ₆ N ₆ /InSe van der Waals Heterostructure: A promising visible-light photocatalyst. <i>Applied Surface Science</i> , 2021, 554, 149465.	3.1	13
43	Charge-compensated codoped pseudo-hexagonal zinc selenide nanosheets towards enhanced visible-light-driven photocatalytic water splitting for hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 34305-34317.	3.8	13
44	<i>R</i> -type LnNiO ₃ (Ln = La, Ce, Nd, Pm, Gd, Tb, Dy, Ho, Er, Lu) half-metals with multiple Dirac cones: a potential class of advanced spintronic materials. <i>IUCr</i> , 2019, 6, 990-995.	1.0	13
45	Visualizing buried silicon atoms at the Cd-Si(111)- interface with localized electrons. <i>Physical Review B</i> , 2017, 96, .		
46	Rotation Tunable Photocatalytic Properties of ZnO/GaN Heterostructures. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900663.	0.7	11
47	Chirality switching of the self-assembled CuPc domains induced by electric field. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7125-7131.	1.3	10
48	First-principles investigation of a new 2D magnetic crystal: Ferromagnetic ordering and intrinsic half-metallicity. <i>Journal of Chemical Physics</i> , 2020, 152, 244704.	1.2	10
49	Density functional calculations for structural, electronic, and magnetic properties of gadolinium-oxide clusters. <i>Journal of Chemical Physics</i> , 2014, 140, .	1.2	9
50	Anion-Doped Monolayer MoS ₂ for Visible Light Photocatalysis. <i>Physica Status Solidi (B): Basic Research</i> , 2018, 255, 1700413.	0.7	9
51	A Hybrid Functional Study on Perovskite-Based Compounds CsPb _{1-x} Sn _x Br ₃ (X = Cl or Br). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5900-5909.	2.1	8
52	Enhancing visible light photocatalytic activity of KNbO ₃ by F passivated co-doping for hydrogen generation by water splitting. <i>Journal of Materials Science</i> , 2017, 52, 5333-5344.	1.7	7
53	Supramolecular Motors on Graphite Surface Stabilized by Charge States and Hydrogen Bonds. <i>ACS Nano</i> , 2017, 11, 10236-10242.	7.3	7
54	Theoretical Insights into Perovskite Compounds MAPb _{1-x} Sn _x I ₃ (X = Ge, Sn; Y = Cl, Br): An Exploration for Superior Optical Performance. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27205-27213.	1.5	7

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55	Study on the hydrogen storage performance of graphene(N)â€“Scâ€“graphene(N) structure. International Journal of Hydrogen Energy, 2020, 45, 33789-33797.	3.8	7
56	Thermoelectric Properties of NiCl ₃ Monolayer: A First-Principles-Based Transport Study. Nanomaterials, 2020, 10, 411.	1.9	7
57	Block elemental-atom-embedded C_3N_4 monolayer with C_3N_4 structure. International Journal of Hydrogen Energy, 2020, 45, 33789-33797.	0.5	6
58	Martensitic transformation, electronic structure and magnetism in D0 ₃ -ordered Heusler Mn ₃ Z (Z = B, Tj) ETQq0 0 0 rgBT /Overlock 10 T. Materials, 2018, 74, 673-680.	0.5	6
59	Thickness and composition dependencies of magnetization and perpendicular magnetic anisotropy of Heusler-like alloys based Mn _x Ga _{1-x} Co ₂ FeAl superlattices. Journal of Alloys and Compounds, 2019, 773, 327-337.	2.8	6
60	Insights into the Microstructures and Energy Levels of Pr ³⁺ -Doped YAlO ₃ Scintillating Crystals. Inorganic Chemistry, 2021, 60, 5107-5113.	1.9	6
61	Exploring the heavy transition metal trihalide family: Two-dimensional magnetic materials with tunable band gap, huge magnetic anisotropy, and high-temperature magnetic ordering. Physical Review Materials, 2022, 6, .	0.9	6
62	Rational design of Mn ₄ GrV ₂ C heterostructures as highly active ORR catalysts: a density functional theory study. RSC Advances, 2022, 12, 14368-14376.	1.7	6
63	Effects of overlayer capping and lattice strain on perpendicular magnetic anisotropy of TM FePt MgO heterostructures. Scientific Reports, 2018, 8, 9429.	1.6	5
64	Band gap and magnetic engineering of penta-graphene <i>via</i> adsorption of small transition clusters. Physical Chemistry Chemical Physics, 2020, 22, 26155-26166.	1.3	5
65	Unveiling the Local Structure and Luminescence Mechanism of Er ³⁺ -Doped LiYF ₄ : A Promising Near-Infrared Laser Crystal. Journal of Physical Chemistry C, 2021, 125, 18015-18021.	1.5	5
66	Emergence of Antiferromagnetic Ordering in Tb _n (n = 2â€“33) Clusters. Journal of Physical Chemistry A, 2014, 118, 1936-1947.	1.1	4
67	2D CdO-Based Heterostructure as a Promising Visible Light Water-Splitting Photocatalyst. Physica Status Solidi (A) Applications and Materials Science, 2020, 217, 1900859.	0.8	4
68	Magnetic moment and magnetic anisotropy of Ge ₃ Mn ₅ thinfilms on Ge(111) substrate: A density functional study. Journal of Chemical Physics, 2018, 148, 074701.	1.2	3
69	Effects of Ga substitution on electronic and thermoelectric properties of gapless semiconductor V ₃ Al. RSC Advances, 2019, 9, 3847-3855.	1.7	3
70	High magnetoresistance and perfect spin filtering effect in silicane/germanene based magnetic Li _{0.5} Cr ₃ Si/Ge Li _{0.5} Cr ₃ tunnel junctions. Journal of Materials Chemistry C, 2021, 9, 13799-13809.	2.7	3
71	Monoxides of small terbium clusters: A density functional theory investigation. Journal of Chemical Physics, 2014, 141, 244304.	1.2	2
72	Deposition Morphology and Magnetism of Co, Pt Adatoms and Small CoPt Adclusters on Ni(100) Substrate. Journal of Cluster Science, 2016, 27, 947-964.	1.7	2

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73	Density functional theory calculations for magnetic properties of Co ₃ W systems. Journal of Chemical Physics, 2018, 149, 014303.	1.2	2
74	Study of photogenerated exciton dissociation in transition metal dichalcogenide van der Waals heterojunction A ₂ MWS ₄ : a first-principles study. Physical Chemistry Chemical Physics, 2021, 23, 26768-26779.	1.3	2
75	Dual-Metal Active Sites Mediated by p-Block Elements: Knowledge-Driven Design of Oxygen Reduction Reaction Catalysts. ACS Omega, 2022, 7, 19676-19686.	1.6	2
76	Electronic, magnetic and optical properties of double perovskite Sr ₂ CuIrO ₆ . European Physical Journal Plus, 2021, 136, 1.	1.2	1
77	Predicted hexagonal titanium nitride monolayer as an intrinsic ferromagnetic semiconductor. EPJ Applied Physics, 2021, 95, 10601.	0.3	1
78	Magnetic properties of Pr bulk and clusters determined using density functional theory calculations. Journal of Magnetism and Magnetic Materials, 2021, 538, 168286.	1.0	0