Huafeng Dong

List of Publications by Citations

62 papers	1,113 citations	17 h-index	32 g-index
71 ext. papers	1,477 ext. citations	5.5 avg, IF	4.66 L-index

#	Paper	IF	Citations
62	Phagraphene: A Low-Energy Graphene Allotrope Composed of 5-6-7 Carbon Rings with Distorted Dirac Cones. *Nano Letters*, **2015**, 15, 6182-6	11.5	325
61	Synergistically Tuning Electronic Structure of Porous Mo2C Spheres by Co Doping and Mo-Vacancies Defect Engineering for Optimizing Hydrogen Evolution Reaction Activity. *Advanced Functional Materials*, **2020**, 30, 2000561	15.6	68
60	The phase diagram and hardness of carbon nitrides. *Scientific Reports*, **2015**, 5, 9870	4.9	66
59	Improving the optical absorption of BiFeO3 for photovoltaic applications via uniaxial compression or biaxial tension. *Applied Physics Letters*, **2013**, 102, 072905	3.4	44
58	New Tungsten Borides, Their Stability and Outstanding Mechanical Properties. *Journal of Physical Chemistry Letters*, **2018**, 9, 3470-3477	6.4	40
57	Novel superhard B-C-O phases predicted from first principles. *Physical Chemistry Chemical Physics*, **2016**, 18, 1859-63	3.6	36
56	Elastic properties of tetragonal BiFeO3 from first-principles calculations. *Applied Physics Letters*, **2013**, 102, 182905	3.4	36
55	Nanotwinned Boron Suboxide (B6O): New Ground State of B6O. *Nano Letters*, **2016**, 16, 4236-42	11.5	35
54	Pressure-induced novel compounds in the Hf-O system from first-principles calculations. *Physical Review B*, **2015**, 92,	3.3	31
53	Trivalent Chromium Ions Doped Fluorides with Both Broad Emission Bandwidth and Excellent Luminescence Thermal Stability. *ACS Applied Materials & Interfaces*, **2021**, 13, 18274-18282	9.5	30
52	Synthesis of Ultra-incompressible sp3-Hybridized Carbon Nitride with 1:1 Stoichiometry. *Chemistry of Materials*, **2016**, 28, 6925-6933	9.6	29
51	Prediction of a new ground state of superhard compound B6O at ambient conditions. *Scientific Reports*, **2016**, 6, 31288	4.9	26
50	Revealing cooperative Li-ion migration in Li1+xAlxTi2(PO4)3 solid state electrolytes with high Al doping. *Journal of Materials Chemistry A*, **2020**, 8, 342-348	13	24
49	First-principles study on strontium titanate for visible light photocatalysis. *Chemical Physics Letters*, **2013**, 555, 141-144	2.5	23
48	Trap Energy Upconversion-Like Near-Infrared to Near-Infrared Light Rejuvenateable Persistent Luminescence. *Advanced Materials*, **2021**, 33, e2008722	24	23
47	Role of defects in enhanced Fermi level pinning at interfaces between metals and transition metal dichalcogenides. *Physical Review B*, **2017**, 96,	3.3	20
46	Unexpected stable phases of tungsten borides. *Physical Chemistry Chemical Physics*, **2018**, 20, 24665-24670	3.6	20

45	Effects of asymmetrical rotated rectangular basis on the acoustic band gap in two-dimensional acoustic crystals: the bands are twisted. *Journal Physics D: Applied Physics*, **2010**, 43, 105404	3	16
44	Superhard conductive orthorhombic carbon polymorphs. *Carbon*, **2020**, 158, 546-552	10.4	16
43	Ratiometric optical thermometer with high sensitivity based on dual far-red emission of Cr3+ in Sr2MgAl22O36. *Ceramics International*, **2020**, 46, 5008-5014	5.1	16
42	Optical anisotropy and blue-shift phenomenon in tetragonal BiFeO3. *Journal Physics D: Applied Physics*, **2013**, 46, 135102	3	15
41	Elastic properties of VO2 from first-principles calculation. *Solid State Communications*, **2013**, 167, 1-4	1.6	14
40	Transition-metal-element dependence of ideal shear strength and elastic behaviors of □-Ni3Al: ab initio study to guide rational alloy design. *Journal of Alloys and Compounds*, **2019**, 806, 1260-1266	5.7	13
39	Unveiling hot carrier relaxation and carrier transport mechanisms in quasi-two-dimensional layered perovskites. *Journal of Materials Chemistry A*, **2020**, 8, 25402-25410	13	13
38	Boron oxides under pressure: Prediction of the hardest oxides. *Physical Review B*, **2018**, 98,	3.3	13
37	First-principles investigation of Zr-O compounds, their crystal structures, and mechanical properties. *Journal of Applied Physics*, **2017**, 121, 155104	2.5	11
36	Understanding the cyan-emitting phosphor RbNa(Li3SiO4)2: Eu2+ by providing Rb ion vacancies. *Journal of Alloys and Compounds*, **2020**, 837, 155084	5.7	9
35	Adsorption mechanism of typical VOCs on pristine and Al-modified MnO2 monolayer. *Applied Surface Science*, **2021**, 539, 148164	6.7	9
34	Toward temperature-dependent Bi3+-related tunable emission in the YVO4:Bi3+ phosphor. *Journal of the American Ceramic Society*, **2019**, 102, 3488-3497	3.8	8
33	Synthesis of submillimeter SnSexS2□ (0 Journal of Materials Chemistry C, **2018**, 6, 4985-4993	7.1	7
32	Na Replaces Rb towards High-Performance Narrow-Band Green Phosphors for Backlight Display Applications. *Advanced Optical Materials*, **2021**, 9, 2100465	8.1	7
31	Novel magnesium borides and their superconductivity. *Physical Chemistry Chemical Physics*, **2017**, 19, 14486-14494	3.6	6
30	Mo-Doped SnO Nanoparticles Embedded in Ultrathin Graphite Nanosheets as a High-Reversible-Capacity, Superior-Rate, and Long-Cycle-Life Anode Material for Lithium-Ion Batteries. *Langmuir*, **2020**, 36, 9276-9283	4	6
29	High-temperature superconductivity in the Ti-H system at high pressures. *Physical Review B*, **2020**, 101,	3.3	6
28	Novel (1 □1)-reconstructions and native defects of TiO2 anatase (101) surface. *Applied Surface Science*, **2017**, 405, 205-208	6.7	5

27	Prediction of new ZnSCaS alloys with anomalous electronic properties. *Journal of Materials Chemistry C*, **2019**, 7, 1246-1254	7.1	5
26	Deep insights into interface engineering by buffer layer for efficient perovskite solar cells: a first-principles study. *Science China Materials*, **2020**, 63, 1588-1596	7.1	3
25	Compressive behavior and elastic properties of Ni-based ternary model superalloys: First-principles calculations and rule of mixtures predications. *Journal of Alloys and Compounds*, **2020**, 839, 155661	5.7	3
24	Na-vacancies-induced magnetism in NaxMnO2. *Journal of Magnetism and Magnetic Materials*, **2018**, 468, 164-167	2.8	3
23	Optical characteristic study of monolayer VS2 based on first-principles calculations. *Solid State Communications*, **2017**, 266, 26-29	1.6	3
22	Exfoliated Graphite Nanosheets Coating on Nano-grained SnO/LiTiO as a High-Performance Anode Material for Lithium-Ion Batteries. *Langmuir*, **2020**, 36, 14666-14675	4	3
21	Vacancies inducing electronic and optical properties in 2D ZnO:Be/Mg. *Physica B: Condensed Matter*, **2019**, 555, 47-52	2.8	3
20	The design of dual-switch fluorescence intensity ratio thermometry with high sensitivity and thermochromism based on a combination strategy of intervalence charge transfer and up-conversion fluorescence thermal enhancement. *Dalton Transactions*, **2021**, 50, 9298-9309	4.3	3
19	A high-density nickel-cobalt alloy embedded in nitrogen-doped carbon nanosheets for the hydrogen evolution reaction.. *Nanoscale*, **2022**,	7.7	3
18	Crystal and band structures of ZnS, MgS, and ZnS-MgS alloys. *Journal of Applied Physics*, **2017**, 121, 235705	2.5	2
17	Photoluminescence properties of Sr2MgSi2O7:Pb2+ and tunable emission from UVB to UVC based on ion substitution. *Journal of Luminescence*, **2020**, 225, 117353	3.8	2
16	A first principles study of p-type doping in two dimensional GaN. *Physical Chemistry Chemical Physics*, **2021**, 23, 20901-20908	3.6	2
15	Factors affecting the negative Poisson's ratio of black phosphorus and black arsenic: electronic effects. *Physical Chemistry Chemical Physics*, **2021**, 23, 3441-3446	3.6	2
14	Orbital localization induced magnetization in nonmetal-doped phosphorene. *Journal Physics D: Applied Physics*, **2020**, 53, 155001	3	1
13	Ferroelectricity and Elasticity of Rhombohedral BiFeO3 Under Uniaxial Stress. *Physica Status Solidi - Rapid Research Letters*, **2018**, 12, 1700431	2.5	1
12	SiC siligraphene: a novel SiC allotrope with wide tunable direct band gap and strong anisotropy. *Journal Physics D: Applied Physics*, **2021**, 54, 225102	3	1
11	Pt/Au surface adsorption on the ZnO surface: A first-principles study. *Solid State Communications*, **2021**, 327, 114204	1.6	1
10	Persistent-Luminescence Phosphors: Trap Energy Upconversion-Like Near-Infrared to Near-Infrared Light Rejuvenateable Persistent Luminescence (Adv. Mater. 15/2021). *Advanced Materials*, **2021**, 33, 2170118	24	1

List of Publications

9	Two-dimensional phosphorus polymorph possessing both wide band gap and strong anisotropy. *Solid State Communications*, **2021**, 114540	1.6	1
8	Pressure-Induced High-Energy-Density BeN4 Materials with Nitrogen Chains: First-Principles Study. *Journal of Physical Chemistry C*, **2021**, 125, 25376-25382	3.8	0
7	Phase Transition and Behaviors of N□N Bonds in Group-IVB Transition-Metal Pernitrides: First-Principles Calculations under High Pressures. *Journal of Physical Chemistry C*, **2021**, 125, 11555-11566	3.8	0
6	Two-dimensional arsenene polymorph beyond the auxetic foam: high mechanical sensitivity and large, negative NPR. *Physical Chemistry Chemical Physics*, **2021**, 23, 3837-3843	3.6	0
5	K replaces Rb towards cyan to red ultra-wideband perovskite-type phosphors for full-spectrum lighting. *Optical Materials*, **2022**, 127, 112246	3.3	0
4	The tunable bandgap of phosphorus-arsenic alloys for mid-and long-infrared regime photodetectors. *Materials Science in Semiconductor Processing*, **2022**, 144, 106552	4.3	0
3	High hardness metal compounds: Prediction of Re3C under pressure. *Applied Physics Letters*, **2021**, 119, 221902	3.4	
2	Rhenium carbides phase diagram under pressure and explaining why WC-type ReC does not exist. *Journal of Applied Physics*, **2022**, 131, 165102	2.5	
1	Graphdiyne@MoS2/WS2 heterostructures for infrared and visible photodetectors: A first-principles study. *Computational Materials Science*, **2022**, 210, 111459	3.2	