

# Qingguo Feng

## List of Publications by Year in descending order

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50  
papers

1,891  
citations

471509

17  
h-index

265206

42  
g-index

50  
all docs

50  
docs citations

50  
times ranked

1913  
citing authors

#	ARTICLE	IF	CITATIONS
1	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	3.0	518
2	Regulating the coordination structure of metal single atoms for efficient electrocatalytic CO <sub>2</sub> reduction. <i>Energy and Environmental Science</i> , 2020, 13, 4609-4624.	30.8	188
3	The most incompressible metal osmium at static pressures above 750 gigapascals. <i>Nature</i> , 2015, 525, 226-229.	27.8	159
4	Quasi-solid-state Zn-air batteries with an atomically dispersed cobalt electrocatalyst and organohydrogel electrolyte. <i>Nature Communications</i> , 2022, 13, .	12.8	127
5	Boosting interfacial charge transfer for alkaline hydrogen evolution via rational interior Se modification. <i>Nano Energy</i> , 2021, 81, 105641.	16.0	118
6	Edge Defect Engineering of Nitrogen-Doped Carbon for Oxygen Electrocatalysts in Zn <sup>2+</sup> /Air Batteries. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 29448-29456.	8.0	110
7	Charge Engineering of Mo <sub>2</sub> C@Defect-Rich N-Doped Carbon Nanosheets for Efficient Electrocatalytic H <sub>2</sub> Evolution. <i>Nano-Micro Letters</i> , 2019, 11, 45.	27.0	86
8	Spin and orbital hybridization at specifically nested Fermi surfaces in URu <sub>2</sub> Si <sub>2</sub> . <i>Physical Review B</i> , 2011, 84, .	3.2	51
9	Rational designed Co@N-doped carbon catalyst for high-efficient H <sub>2</sub> S selective oxidation by regulating electronic structures. <i>Chemical Engineering Journal</i> , 2020, 401, 126038.	12.7	43
10	Enhanced Selective H <sub>2</sub> S Oxidation Performance on Mo <sub>2</sub> C-Modified g-C <sub>3</sub> N <sub>4</sub> . <i>ACS Sustainable Chemistry and Engineering</i> , 2019, 7, 16257-16263.	6.7	39
11	Accelerating charge transfer to enhance H <sub>2</sub> evolution of defect-rich CoFe <sub>2</sub> O <sub>4</sub> by constructing a Schottky junction. <i>Chemical Communications</i> , 2020, 56, 14019-14022.	4.1	34
12	Synthesis and characterization of ternary layered Nb <sub>2</sub> SB ceramics fabricated by spark plasma sintering. <i>Journal of Alloys and Compounds</i> , 2021, 878, 160344.	5.5	25
13	Achieving Predictive Description of Molecular Conductance by Using a Range-Separated Hybrid Functional. <i>Nano Letters</i> , 2016, 16, 6092-6098.	9.1	21
14	Modification of Molecular Conductance by in Situ Deprotection of Thiol-Based Porphyrin. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 15901-15906.	8.0	20
15	Design, fabrication, microstructure, and properties of highly porous alumina whisker foam ceramic. <i>Ceramics International</i> , 2022, 48, 2776-2781.	4.8	20
16	Synthesis and property characterization of ternary laminar Zr <sub>2</sub> SB ceramic. <i>Journal of Advanced Ceramics</i> , 2022, 11, 825-833.	17.4	20
17	The functionality of surface hydroxyls on selective CH <sub>4</sub> generation from photoreduction of CO <sub>2</sub> over SiC nanosheets. <i>Chemical Communications</i> , 2019, 55, 1572-1575.	4.1	19
18	Comparative study of perovskite-type scintillator materials CsCa <sub>3</sub> and KCa <sub>3</sub> via first-principles calculations. <i>Journal Physics D: Applied Physics</i> , 2018, 51, 065303.	2.8	18

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19	Ablation behavior and mechanism of bulk MoAlB ceramic at $\frac{1}{4}$ 1670 $\pm$ 2550 $\text{\AA}^\circ\text{C}$ in air plasma flame. Journal of the European Ceramic Society, 2021, 41, 5474-5483.	5.7	18
20	Fast impurity solver based on equations of motion and decoupling. Physical Review B, 2009, 79, .	3.2	17
21	Structural engineering of bilayer PtSe <sub>2</sub> thin films: a first-principles study. Journal of Physics Condensed Matter, 2019, 31, 455001.	1.8	16
22	Anisotropic distortion and Lifshitz transition in $\text{Hf}$ under pressure. Physical Review B, 2017, 95, .	3.2	14
23	Preparations and Applications of MXene $\rightarrow$ Metal Composites: A Review. Coatings, 2022, 12, 516.	2.6	14
24	Tunable electronic properties of monolayer MnPSe <sub>3</sub> /MoTe <sub>2</sub> heterostructure: a first principles study. Journal of Physics Condensed Matter, 2019, 31, 405705.	1.8	13
25	Stress $\rightarrow$ Driven Phase Transitions of Sr <sub>2</sub> : A First $\rightarrow$ Principles Investigation. Physica Status Solidi (B): Basic Research, 2020, 257, 1900726.	1.5	13
26	Conductance of Junctions with Acetyl-Functionalized Thiols: A First-Principles-Based Analysis. Journal of Physical Chemistry C, 2017, 121, 10298-10304.	3.1	12
27	Field controllable electronic properties of MnPSe <sub>3</sub> /WS <sub>2</sub> heterojunction for photocatalysis. Journal of Central South University, 2021, 28, 3728-3736.	3.0	11
28	Deleterious Effects of Exact Exchange Functionals on Predictions of Molecular Conductance. Journal of Chemical Theory and Computation, 2016, 12, 3431-3435.	5.3	10
29	Topological transitions of the Fermi surface of osmium under pressure: an LDA+DMFT study. New Journal of Physics, 2017, 19, 033020.	2.9	10
30	Theoretical Investigation on Hydrogen Abstraction by NO <sub>2</sub> from Symmetric Ethers (CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> O ( $\chi = 1\text{\AA}^4$ ). Journal of Physical Chemistry A, 2018, 122, 6829-6841.	2.5	10
31	Thickness-dependent ultrafast hot carrier and phonon dynamics of PtSe <sub>2</sub> films measured with femtosecond transient optical spectroscopy. Journal Physics D: Applied Physics, 2021, 54, 075102.	2.8	10
32	Rapidly synthesizing Hf <sub>2</sub> SB ceramics by thermal explosion. Journal of the European Ceramic Society, 2022, 42, 3780-3786.	5.7	10
33	Emerging New Pseudobinary and Ternary Halides as Scintillators for Radiation Detection. IEEE Transactions on Nuclear Science, 2017, 64, 1817-1824.	2.0	9
34	Comparative investigation of ultrafast thermal shock of Ti <sub>3</sub> AlC <sub>2</sub> ceramic in water and air. International Journal of Applied Ceramic Technology, 2021, 18, 1863-1871.	2.1	9
35	First principles investigation of electron correlation and Lifshitz transition within iron polynitrides. Journal of Physics Condensed Matter, 2021, 33, 035603.	1.8	9
36	Investigation of double perovskites Sr <sub>2</sub> SmNbO <sub>6</sub> and X <sub>2</sub> CoNbO <sub>6</sub> (X=Sr,Ba) with SCAN functional and plus U correction. , 2022, 1, 100019.		9

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37	Electronic, magnetic and optical properties of transition-metal and hydroxides doped monolayer $g\text{-C}_{3\text{N}_4}$ : a first principles investigation. Journal of Physics Condensed Matter, 2020, 32, 445602.	1.8	8
38	Ramifications of codoping $\text{SrI}_2\text{:Eu}$ with isovalent and aliovalent impurities. Journal of Applied Physics, 2016, 120, 213104.	2.5	7
39	Electron correlation effect versus spin-orbit coupling for tungsten and impurities. Journal of Physics Condensed Matter, 2020, 32, 445603.	1.8	7
40	An advanced multi-orbital impurity solver for dynamical mean field theory based on the equation of motion approach. Journal of Physics Condensed Matter, 2012, 24, 055603.	1.8	5
41	A magnetically controllable metastable $\text{LiSeHFeO}$ isomer: an ab-initio investigation from bulk to film. Journal of Materials Science, 2021, 56, 1461-1471.	3.7	5
42	Behavior of intrinsic defects in $\text{BaF}_2$ under uniaxial compressions: An ab initio investigation. Materials Today Communications, 2021, 28, 102730.	1.9	5
43	Ablation mechanisms of $\text{Ti}_3\text{SiC}_2$ ceramic at $1600\text{ }^\circ\text{C}$ in nitrogen plasma flame. Ceramics International, 2022, 48, 14004-14013.	4.8	5
44	Fast multi-orbital equation of motion impurity solver for dynamical mean field theory. Journal of Physics Condensed Matter, 2011, 23, 425601.	1.8	4
45	Investigation of on-site interorbital single-electron hoppings in general multiorbital systems. Physical Review B, 2012, 86, .	3.2	4
46	The role of hydroxyl groups in interchain interactions in cellulose $\text{I}_{\beta}$ and $\text{I}_{\gamma}$ . International Journal of Quantum Chemistry, 2017, 117, e25357.	2.0	4
47	Fabrication, Microstructure, and Properties of In Situ $\text{V}_2\text{C}$ -Reinforced Copper Composites. Metals, 2021, 11, 1829.	2.3	3
48	Hydrogen abstraction by $\text{NO}_2$ from asymmetric methyl ethers: A theoretical investigation. Chemical Physics Letters, 2018, 710, 133-142.	2.6	2
49	Electronic, optical properties and stress-driven modulation of monolayer $\text{MNb}_3\text{O}_8$ ( $\text{M}=\text{H, Li, Na, K}$ ): An ab-initio investigation. Materials Today Communications, 2021, 26, 101867.	1.9	2
50	Synthesis of $\text{Al}_2\text{O}_3$ Whiskers with Twins. Metals, 2021, 11, 895.	2.3	0