Pengyue Gao

List of Publications by Year
in descending order

21	467	933447 10	752698 20
papers	citations	h-index	g-index

21	21	21	463
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Interface structure prediction via CALYPSO method. Science Bulletin, 2019, 64, 301-309.	9.0	219
2	Combining Machine Learning Potential and Structure Prediction for Accelerated Materials Design and Discovery. Journal of Physical Chemistry Letters, 2020, 11, 8710-8720.	4.6	45
3	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	3.0	40
4	X-ray diffraction data-assisted structure searches. Computer Physics Communications, 2017, 213, 40-45.	7.5	30
5	The CALYPSO methodology for structure prediction*. Chinese Physics B, 2019, 28, 106105.	1.4	28
6	Machine learning metadynamics simulation of reconstructive phase transition. Physical Review B, 2021, 103, .	3.2	15
7	Disproportionation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> at High Pressure and Temperature. Physical Review Letters, 2022, 128, 106001.	7.8	13
8	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	8.7	12
9	Ab initio electronic structure calculations using a real-space Chebyshev-filtered subspace iteration method. Journal of Physics Condensed Matter, 2019, 31, 455901.	1.8	11
10	Structure search of two-dimensional systems using CALYPSO methodology. Frontiers of Physics, 2022, 17, 1.	5.0	11
11	A database assisted protein structure prediction method via a swarm intelligence algorithm. RSC Advances, 2017, 7, 39869-39876.	3.6	7
12	Ironâ€“magnesium compounds under high pressure. New Journal of Chemistry, 2019, 43, 17403-17407.	2.8	7
13	The superconductivity of Nâ€“Siâ€“H compounds at high pressure. Solid State Communications, 2021, 329, 114260.	1.9	6
14	Stabilization of S3O4 at high pressure: implications for the sulfur-excess paradox. Science Bulletin, 2022, 67, 971-976.	9.0	6
15	Pressure-stabilized high-energy-density material YN₁₀. Journal of Physics Condensed Matter, 2022, 34, 135403.	1.8	5
16	Phase transition and electronic properties of barium fluoride at high pressure. Solid State Communications, 2022, 342, 114597.	1.9	4
17	High-pressure modulated structures in beryllium chalcogenides. Physical Review B, 2019, 100, .	3.2	3
18	Stability of Ca(OH)2 at Earth's deep lower mantle conditions. Physical Review B, 2021, 104, .	3.2	2

#	Article	IF	Citations
19	Synthesis of calcium polysulfides at high pressures. Physical Review B, 2021, 104, .	3.2	2
20	Pressure-induced formation of bulk Ge-Sn compounds with high concentration of Sn. Solid State Communications, 2019, 293, 48-52.	1.9	1
21	Semiconducting <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ba</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> phase featuring ν-shape <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> unit at high pressure. Physical Review Research, 2022, 4, .	3.6	0