## Shoutao Zhang

## List of Publications by Citations

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#	Paper	IF	Citations
42	TiC Monolayer with High Specific Capacity for Sodium-Ion Batteries. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 5962-5968	16.4	152
41	Tellurium Hydrides at High Pressures: High-Temperature Superconductors. <i>Physical Review Letters</i> , <b>2016</b> , 116, 057002	7.4	104
40	Two-Dimensional PC with Direct Band Gap and Anisotropic Carrier Mobility. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 1599-1605	16.4	76
39	Phase Diagram and High-Temperature Superconductivity of Compressed Selenium Hydrides. <i>Scientific Reports</i> , <b>2015</b> , 5, 15433	4.9	56
38	Predicted Pressure-Induced Superconducting Transition in Electride Li_{6}P. <i>Physical Review Letters</i> , <b>2019</b> , 122, 097002	7.4	51
37	High-Temperature Ferromagnetism in an FeP Monolayer with a Large Magnetic Anisotropy. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2733-2738	6.4	50
36	Gold with +4 and +6 Oxidation States in AuF and AuF. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 9545-9550	16.4	50
35	Stable and metallic two-dimensional TaC2 as an anode material for lithium-ion battery. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 18698-18706	13	50
34	Metallic P3C monolayer as anode for sodium-ion batteries. <i>Journal of Materials Chemistry A</i> , <b>2019</b> , 7, 405-411	13	49
33	Structure and Electronic Properties of FeSH Compound under High Pressure. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 11434-11439	5.1	35
32	Understanding the role of lithium sulfide clusters in lithiumBulfur batteries. <i>Journal of Materials Chemistry A</i> , <b>2017</b> , 5, 9293-9298	13	34
31	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. <i>Computer Physics Communications</i> , <b>2016</b> , 200, 87-95	4.2	29
30	Pressure-induced stable BeN 4 as a high-energy density material. <i>Journal of Power Sources</i> , <b>2017</b> , 365, 155-161	8.9	22
29	Nonmetallic FeH6 under High Pressure. Journal of Physical Chemistry C, 2018, 122, 12022-12028	3.8	21
28	Phase diagram, stability and electronic properties of an Fe <b>P</b> system under high pressure: a first principles study. <i>RSC Advances</i> , <b>2017</b> , 7, 15986-15991	3.7	18
27	Pressure-Induced Stable Beryllium Peroxide. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 5233-5238	5.1	15
26	Hexagonal BC2N with Remarkably High Hardness. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 6801-6807	3.8	15

## (2020-2016)

25	First-principle optimal local pseudopotentials construction via optimized effective potential method. <i>Journal of Chemical Physics</i> , <b>2016</b> , 144, 134108	3.9	15
24	Exploring High-Pressure Structures of N2CO. <i>Journal of Physical Chemistry C</i> , <b>2014</b> , 118, 27252-27257	3.8	13
23	Crystal Structures and Electronic Properties of Cesium Xenides at High Pressures. <i>Journal of Physical Chemistry C</i> , <b>2015</b> , 119, 24996-25002	3.8	12
22	Ten-fold coordinated polymorph and metallization of TiO2 under high pressure. <i>RSC Advances</i> , <b>2015</b> , 5, 54253-54257	3.7	11
21	Silicon Framework-Based Lithium Silicides at High Pressures. <i>ACS Applied Materials &amp; Discourse (Control of the Control of the</i>	9.5	11
20	Superconducting boron allotropes. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	8
19	Hypervalent Iodine with Linear Chain at High Pressure. Scientific Reports, 2015, 5, 14393	4.9	8
18	Phase diagrams and electronic properties of B-S and H-B-S systems under high pressure. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	7
17	Hard and superconducting cubic boron phase via swarm-intelligence structural prediction driven by a machine-learning potential. <i>Physical Review B</i> , <b>2021</b> , 103,	3.3	7
16	Unveiling the Role of Oxygen Vacancy in Li2MnO3 upon Delithiation. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 23403-23409	3.8	6
15	Globally stable structures of LixZn ( $x = 1-4$ ) compounds at high pressures. <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 4437-43	3.6	6
14	Tetragonal Structure BC4 as a Superhard Material. <i>Journal of Physical Chemistry C</i> , <b>2017</b> , 121, 10119-10	1338	5
13	Structural and Superconducting Properties of Tungsten Hydrides Under High Pressure. <i>Frontiers in Physics</i> , <b>2018</b> , 6,	3.9	5
12	Exploring the metallic phase of N2O under high pressure. <i>RSC Advances</i> , <b>2015</b> , 5, 65745-65749	3.7	4
11	Pressure-induced structural changes and elemental dissociation of cadmium and mercury chalcogenides. <i>RSC Advances</i> , <b>2015</b> , 5, 104426-104432	3.7	4
10	Achieving high hydrogen evolution reaction activity of a MoC monolayer. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 26189-26199	3.6	4
9	Fabrication of Alkali Metal Boride: Honeycomb-Like Structured NaB4 with High Hardness and Excellent Electrical Conductivity. <i>Advanced Functional Materials</i> ,2110872	15.6	2
8	Structural and electronic properties of tungsten oxides under high pressures. <i>Journal of Physics Condensed Matter</i> , <b>2020</b> , 32, 085403	1.8	2

7	Superconductive Sodium Carbides with Pentagon Carbon at High Pressures. <i>Journal of Physical Chemistry Letters</i> , <b>2021</b> , 12, 5850-5856	6.4	2
6	Pressure-stabilized GdN6 with an armchairਬntiarmchair structure as a high energy density material. <i>Journal of Materials Chemistry A</i> , <b>2021</b> , 9, 16751-16758	13	2
5	Multi-mode plasmonic resonance broadband LWIR metamaterial absorber based on lossy metal ring <i>Optics Express</i> , <b>2022</b> , 30, 473-483	3.3	2
4	Unconventional stable stoichiometry of vanadium peroxide. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 11460-11466	3.6	1
3	Crystal structures and superconductivity of lithium and fluorine implanted gold hydrides under high pressures. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 21544-21553	3.6	1
2	Emerging Yttrium Phosphides with Tetrahedron Phosphorus and Superconductivity under High Pressures. <i>Chemistry - A European Journal</i> , <b>2021</b> , 27, 17420-17427	4.8	O
1	Pressure-Driven Ne-Bearing Polynitrides with Ultrahigh Energy Density. <i>Chinese Physics Letters</i> , <b>2022</b> , 39, 056102	1.8	О