

# Zeyu Deng

## List of Publications by Year in descending order

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25  
papers

1,782  
citations

471509

17  
h-index

642732

23  
g-index

33  
all docs

33  
docs citations

33  
times ranked

2251  
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards autonomous high-throughput multiscale modelling of battery interfaces. Energy and Environmental Science, 2022, 15, 579-594.	30.8	17
2	Superionic Conduction in the Plastic Crystal Polymorph of Na <sub>4</sub> P <sub>2</sub> S <sub>6</sub> . ACS Energy Letters, 2022, 7, 1403-1411.	17.4	9
3	Crystal Structure of Na <sub>2</sub> V <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> , an Intriguing Phase Spotted in the Na <sub>3</sub> V <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> –Na <sub>1</sub> V <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> System. Chemistry of Materials, 2022, 34, 451-462.	6.7	31
4	Unlocking the origin of compositional fluctuations in InGaN light emitting diodes. Physical Review Materials, 2021, 5, .	2.4	7
5	(Invited) Revisiting the Structure–Property Relationships in NaSICON Electrode and Electrolytes. ECS Meeting Abstracts, 2021, MA2021-01, 456-456.	0.0	0
6	Slow carrier relaxation in tin-based perovskite nanocrystals. Nature Photonics, 2021, 15, 696-702.	31.4	40
7	Phase stability and sodium-vacancy orderings in a NaSICON electrode. Journal of Materials Chemistry A, 2021, 10, 209-217.	10.3	24
8	Phase Behavior in Rhombohedral NaSICON Electrolytes and Electrodes. Chemistry of Materials, 2020, 32, 7908-7920.	6.7	58
9	Halogenated Metal–Organic Framework Glasses and Liquids. Journal of the American Chemical Society, 2020, 142, 3880-3890.	13.7	83
10	Understanding the Structural and Electronic Properties of Bismuth Trihalides and Related Compounds. Inorganic Chemistry, 2020, 59, 3377-3386.	4.0	9
11	Metal-free perovskites for non linear optical materials. Chemical Science, 2019, 10, 8187-8194.	7.4	46
12	Improving the Acidic Stability of Zeolitic Imidazolate Frameworks by Biofunctional Molecules. Chem, 2019, 5, 1597-1608.	11.7	148
13	<i>Ab initio</i> computation for solid-state <sup>31</sup> P NMR of inorganic phosphates: revisiting X-ray structures. Physical Chemistry Chemical Physics, 2019, 21, 10070-10074.	2.8	10
14	Enhanced visible light absorption for lead-free double perovskite Cs <sub>2</sub> AgSbBr <sub>6</sub> . Chemical Communications, 2019, 55, 3721-3724.	4.1	117
15	Polymorphism in M(H <sub>2</sub> PO <sub>2</sub> ) <sub>3</sub> (M = V, Al, Ga) compounds with the perovskite-related ReO <sub>3</sub> structure. Chemical Communications, 2019, 55, 2964-2967.	4.1	15
16	Elastic properties and thermal expansion of lead-free halide double perovskite Cs <sub>2</sub> AgBiBr <sub>6</sub> . Computational Materials Science, 2018, 141, 49-58.	3.0	87
17	The competition between mechanical stability and charge carrier mobility in MA-based hybrid perovskites: insight from DFT. Journal of Materials Chemistry C, 2018, 6, 12252-12259.	5.5	42
18	Octahedral connectivity and its role in determining the phase stabilities and electronic structures of low-dimensional, perovskite-related iodoplumbates. APL Materials, 2018, 6, .	5.1	23

#	ARTICLE	IF	CITATIONS
19	Synthesis and Properties of a Lead-Free Hybrid Double Perovskite: $(\text{CH}_3\text{NH}_3)_2\text{AgBiBr}_6$ . Chemistry of Materials, 2017, 29, 1089-1094.	6.7	290
20	Variable temperature and high-pressure crystal chemistry of perovskite formamidinium lead iodide: a single crystal X-ray diffraction and computational study. Chemical Communications, 2017, 53, 7537-7540.	4.1	43
21	Factors Influencing the Mechanical Properties of Formamidinium Lead Halides and Related Hybrid Perovskites. ChemSusChem, 2017, 10, 3683-3683.	6.8	0
22	Synthesis and Characterization of the Rare-Earth Hybrid Double Perovskites: $(\text{CH}_3\text{NH}_3)_2\text{KGdCl}_6$ and $(\text{CH}_3\text{NH}_3)_2\text{KYCl}_6$ . Journal of Physical Chemistry Letters, 2017, 8, 5015-5020.	4.6	68
23	Factors Influencing the Mechanical Properties of Formamidinium Lead Halides and Related Hybrid Perovskites. ChemSusChem, 2017, 10, 3740-3745.	6.8	80
24	The synthesis, structure and electronic properties of a lead-free hybrid inorganic-organic double perovskite $(\text{MA})_2\text{KBiCl}_6$ (MA = methylammonium). Materials Horizons, 2016, 3, 328-332.	12.2	284
25	Exploring the properties of lead-free hybrid double perovskites using a combined computational-experimental approach. Journal of Materials Chemistry A, 2016, 4, 12025-12029.	10.3	250