

Tran Doan Huan

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

84
papers

3,165
citations

29
h-index

55
g-index

90
ext. papers

3,928
ext. citations

6.4
avg, IF

5.81
L-index

#	Paper	IF	Citations
84	Mesoporous MoO ₃ xH ₂ O Material as an Efficient Electrocatalyst for Hydrogen Evolution Reactions. <i>Advanced Energy Materials</i> , 2016 , 6, 1600528	21.8	262
83	Pathways towards ferroelectricity in hafnia. <i>Physical Review B</i> , 2014 , 90,	3.3	230
82	Machine Learning Strategy for Accelerated Design of Polymer Dielectrics. <i>Scientific Reports</i> , 2016 , 6, 20952	4.9	207
81	Advanced polymeric dielectrics for high energy density applications. <i>Progress in Materials Science</i> , 2016 , 83, 236-269	42.2	193
80	Polymer Genome: A Data-Powered Polymer Informatics Platform for Property Predictions. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 17575-17585	3.8	156
79	A universal strategy for the creation of machine learning-based atomistic force fields. <i>Npj Computational Materials</i> , 2017 , 3,	10.9	155
78	Rational Co-Design of Polymer Dielectrics for Energy Storage. <i>Advanced Materials</i> , 2016 , 28, 6277-91	24	118
77	Accelerated materials property predictions and design using motif-based fingerprints. <i>Physical Review B</i> , 2015 , 92,	3.3	111
76	Factors Favoring Ferroelectricity in Hafnia: A First-Principles Computational Study. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 4139-4145	3.8	105
75	A polymer dataset for accelerated property prediction and design. <i>Scientific Data</i> , 2016 , 3, 160012	8.2	100
74	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. <i>Materials Today</i> , 2018 , 21, 785-796	21.8	99
73	Dopants Promoting Ferroelectricity in Hafnia: Insights from a comprehensive Chemical Space Exploration. <i>Chemistry of Materials</i> , 2017 , 29, 9102-9109	9.6	87
72	Stabilization of metastable phases in hafnia owing to surface energy effects. <i>Applied Physics Letters</i> , 2016 , 108, 172902	3.4	74
71	A hybrid organic-inorganic perovskite dataset. <i>Scientific Data</i> , 2017 , 4, 170057	8.2	73
70	Interlayer Interactions in van der Waals Heterostructures: Electron and Phonon Properties. <i>ACS Applied Materials & Interfaces</i> , 2016 , 8, 6286-92	9.5	53
69	Poly(dimethyltin glutarate) as a prospective material for high dielectric applications. <i>Advanced Materials</i> , 2015 , 27, 346-51	24	52
68	Machine learning models for the lattice thermal conductivity prediction of inorganic materials. <i>Computational Materials Science</i> , 2019 , 170, 109155	3.2	49

67	Rational Design of Organotin Polyesters. <i>Macromolecules</i> , 2015 , 48, 2422-2428	5.5	47
66	Polymer design using genetic algorithm and machine learning. <i>Computational Materials Science</i> , 2021 , 186, 110067	3.2	43
65	Activating low-temperature diesel oxidation by single-atom Pt on TiO nanowire array. <i>Nature Communications</i> , 2020 , 11, 1062	17.4	42
64	Charge injection barriers at metal/polyethylene interfaces. <i>Journal of Materials Science</i> , 2016 , 51, 506-512	7.3	42
63	Role of Oxygen Vacancy Defects in the Electrocatalytic Activity of Substoichiometric Molybdenum Oxide. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 18212-18222	3.8	42
62	Novel structural motifs in low energy phases of LiAlH ₄ . <i>Physical Review Letters</i> , 2012 , 108, 205505	7.4	42
61	Machine-learning predictions of polymer properties with Polymer Genome. <i>Journal of Applied Physics</i> , 2020 , 128, 171104	2.5	41
60	Mining Materials Design Rules from Data: The Example of Polymer Dielectrics. <i>Chemistry of Materials</i> , 2017 , 29, 9001-9010	9.6	36
59	Frequency-dependent dielectric constant prediction of polymers using machine learning. <i>Npj Computational Materials</i> , 2020 , 6,	10.9	35
58	Electronic Structure of Polyethylene: Role of Chemical, Morphological and Interfacial Complexity. <i>Scientific Reports</i> , 2017 , 7, 6128	4.9	34
57	Low-energy polymeric phases of alanates. <i>Physical Review Letters</i> , 2013 , 110, 135502	7.4	33
56	Polymer informatics: Current status and critical next steps. <i>Materials Science and Engineering Reports</i> , 2021 , 144, 100595	30.9	33
55	Layered structures of organic/inorganic hybrid halide perovskites. <i>Physical Review B</i> , 2016 , 93,	3.3	29
54	Thermodynamic stability of alkali-metal zinc double-cation borohydrides at low temperatures. <i>Physical Review B</i> , 2013 , 88,	3.3	27
53	A multi-fidelity information-fusion approach to machine learn and predict polymer bandgap. <i>Computational Materials Science</i> , 2020 , 172, 109286	3.2	27
52	Polyelectrolyte-Assisted Oxygen Vacancies: A New Route to Defect Engineering in Molybdenum Oxide. <i>Langmuir</i> , 2018 , 34, 6296-6306	4	26
51	Tunable Spin-Dependent Properties of Zigzag Silicene Nanoribbons. <i>Physical Review Applied</i> , 2014 , 1,	4.3	26
50	Effect of incorporating aromatic and chiral groups on the dielectric properties of poly(dimethyltin esters). <i>Macromolecular Rapid Communications</i> , 2014 , 35, 2082-8	4.8	26

49	Low-energy structures of zinc borohydride Zn(BH ₄) ₂ . <i>Physical Review B</i> , 2012 , 86,	3.3	26
48	General Atomic Neighborhood Fingerprint for Machine Learning-Based Methods. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 15859-15866	3.8	23
47	High-pressure phases of Mg ₂ Si from first principles. <i>Physical Review B</i> , 2016 , 93,	3.3	23
46	Polymers for Extreme Conditions Designed Using Syntax-Directed Variational Autoencoders. <i>Chemistry of Materials</i> , 2020 , 32, 10489-10500	9.6	21
45	Unraveling the luminescence signatures of chemical defects in polyethylene. <i>Journal of Chemical Physics</i> , 2015 , 143, 124907	3.9	21
44	Block Copolymer-Assisted Solvothermal Synthesis of Hollow BiMoO Spheres Substituted with Samarium. <i>Langmuir</i> , 2016 , 32, 10967-10976	4	21
43	Roughness-induced piezoelectric scattering in lattice-mismatched semiconductor quantum wells. <i>Physical Review B</i> , 2003 , 68,	3.3	19
42	Random piezoelectric field in real [001]-oriented strain-relaxed semiconductor heterostructures. <i>Physical Review Letters</i> , 2002 , 89, 077601	7.4	19
41	Iterative-Learning Strategy for the Development of Application-Specific Atomistic Force Fields. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 20715-20722	3.8	18
40	First-principles predicted low-energy structures of NaSc(BH ₄) ₄ . <i>Journal of Chemical Physics</i> , 2014 , 140, 124708	3.9	17
39	Low-temperature mobility of holes in Si _{0.5} Bi _{0.5} Ge p-channel heterostructures. <i>Physical Review B</i> , 2004 , 70,	3.3	16
38	Exploring PtSO ₄ and PdSO ₄ phases: an evolutionary algorithm based investigation. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 18146-51	3.6	13
37	Polymer Structure Prediction from First Principles. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5823-5829	3.4	11
36	Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 37182-37187	9.5	11
35	Theoretical prediction of low-density hexagonal ZnO hollow structures. <i>Journal of Applied Physics</i> , 2016 , 120, 142105	2.5	11
34	Strain fluctuations in a real [001]-oriented zinc-blende-structure surface quantum well. <i>Physical Review B</i> , 2003 , 68,	3.3	10
33	Atomistic mechanisms for chemical defects formation in polyethylene. <i>Journal of Chemical Physics</i> , 2018 , 149, 234902	3.9	10
32	Valence bond entanglement and fluctuations in random singlet phases. <i>Physical Review B</i> , 2011 , 84,	3.3	9

31	Pressure-stabilized binary compounds of magnesium and silicon. <i>Physical Review Materials</i> , 2018 , 2, 3.2	9
30	Computational predictions of zinc oxide hollow structures. <i>Physica B: Condensed Matter</i> , 2018 , 532, 15-19.8	7
29	Modeling study on the properties of GaN/AlN core/shell nanowires by surface effect suppression. <i>Physica Status Solidi (B): Basic Research</i> , 2012 , 249, 1241-1249	1.3 7
28	Polymer informatics with multi-task learning. <i>Patterns</i> , 2021 , 2, 100238	5.1 7
27	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 3937-3943	6.4 6
26	Compositional Effects and Electron Lone-pair Distortions in Doped Bournonites. <i>ChemPhysChem</i> , 2018 , 19, 2635-2644	3.2 5
25	Predicted Binary Compounds of Tin and Sulfur. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 17067-17072	3.8 5
24	Cage disorder and gas encapsulation as routes to tailor properties of inorganic clathrates. <i>Acta Materialia</i> , 2017 , 131, 475-481	8.4 5
23	Size-induced structural transition in ZnO prismatic nanoparticles. <i>Physica Status Solidi (B): Basic Research</i> , 2012 , 249, 535-543	1.3 5
22	Monte Carlo simulations of interacting anyon chains. <i>Computational Materials Science</i> , 2010 , 49, S395-S398	3.8 5
21	Dielectric Polymers Tolerant to Electric Field and Temperature Extremes: Integration of Phenomenology, Informatics, and Experimental Validation. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 53416-53424	9.5 5
20	Density functional theory based tight binding study on theoretical prediction of low-density nanoporous phases ZnO semiconductor materials. <i>Journal of Physics: Conference Series</i> , 2016 , 726, 012022	0.3 4
19	First-principles prediction for the stability of LiK. <i>Physica Status Solidi (B): Basic Research</i> , 2014 , 251, 1539-1544	1.3 4
18	polyG2G: A Novel Machine Learning Algorithm Applied to the Generative Design of Polymer Dielectrics. <i>Chemistry of Materials</i> , 2021 , 33, 7008-7016	9.6 4
17	Novel cage-like nanoporous ZnO polymorphs with cubic lattice frameworks. <i>Materials Today Communications</i> , 2020 , 24, 101152	2.5 3
16	Thermal transport in phase-stabilized lithium zirconate phosphates. <i>Applied Physics Letters</i> , 2020 , 117, 011903	3.4 3
15	Lead-free hybrid organic-inorganic perovskites for solar cell applications. <i>Journal of Chemical Physics</i> , 2020 , 152, 014104	3.9 3
14	Search for Ferroelectric Binary Oxides: Chemical and Structural Space Exploration Guided by Group Theory and Computations. <i>Chemistry of Materials</i> , 2020 , 32, 3823-3832	9.6 3

13	Novel high voltage polymer insulators using computational and data-driven techniques. <i>Journal of Chemical Physics</i> , 2021 , 154, 174906	3.9	3
12	Characterizing magnesium-silicon binaries in AlMgSi supersaturated solid solution by first-principles calculations. <i>Journal of Science: Advanced Materials and Devices</i> , 2016 , 1, 527-530	4.2	3
11	An Efficient Deep Learning Scheme To Predict the Electronic Structure of Materials and Molecules: The Example of Graphene-Derived Allotropes. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 9496-9502	2.8	2
10	Impact of Surface on the d^0 Ferromagnetism of Lithium-Doped Zinc Oxide Nanowires. <i>IEEE Transactions on Magnetics</i> , 2014 , 50, 1-7	2	2
9	Diffusion thermopower of a p-type Si/Si _{1-x} Ge _x heterostructure at zero magnetic field. <i>Physica Status Solidi (B): Basic Research</i> , 2007 , 244, 2100-2108	1.3	1
8	Effect of impurity correlation in modulation-doped quantum wires. <i>Physical Review B</i> , 2001 , 64,	3.3	1
7	Strong Rashba-Dresselhaus Effect in Nonchiral 2D Ruddlesden-Popper Perovskites. <i>Advanced Optical Materials</i> , 2101232	8.1	1
6	Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries.. <i>Journal of Chemical Theory and Computation</i> , 2022 ,	6.4	1
5	Toward Recyclable Polymers: Ring-Opening Polymerization Enthalpy from First-Principles. <i>Journal of Physical Chemistry Letters</i> , 4778-4785	6.4	1
4	Structural, Electronic and Mechanical Properties of Few-Layer GaN Nanosheet: A First-Principle Study. <i>Materials Transactions</i> , 2020 , 61, 1438-1444	1.3	0
3	Atomic configurations for materials research: A case study of some simple binary compounds. <i>AIP Advances</i> , 2021 , 11, 045120	1.5	0
2	High dielectric constant and high breakdown strength polyimide tin complexation of the polyamide acid precursor.. <i>RSC Advances</i> , 2022 , 12, 9095-9100	3.7	0
1	Highly charged interface trap states in PbS _{1-x} govern electro-thermal transport. <i>APL Materials</i> , 2019 , 7, 071105	5.7	