Tran Doan Huan

List of Publications by Year
in descending order

88 papers	4,767 citations	126858 33 h-index	95218 68 g-index
90 all docs	90 docs citations	90 times ranked	4951 citing authors

#	Article	IF	Citations
1	Mesoporous MoO_{3â€“}_x Material as an Efficient Electrocatalyst for Hydrogen Evolution Reactions. Advanced Energy Materials, 2016, 6, 1600528.	10.2	353
2	Pathways towards ferroelectricity in hafnia. Physical Review B, 2014, 90, .	1.1	351
3	Advanced polymeric dielectrics for high energy density applications. Progress in Materials Science, 2016, 83, 236-269.	16.0	286
4	Machine Learning Strategy for Accelerated Design of Polymer Dielectrics. Scientific Reports, 2016, 6, 20952.	1.6	279
5	Polymer Genome: A Data-Powered Polymer Informatics Platform for Property Predictions. Journal of Physical Chemistry C, 2018, 122, 17575-17585.	1.5	271
6	A universal strategy for the creation of machine learning-based atomistic force fields. Npj Computational Materials, 2017, 3, .	3.5	188
7	Factors Favoring Ferroelectricity in Hafnia: A First-Principles Computational Study. Journal of Physical Chemistry C, 2017, 121, 4139-4145.	1.5	158
8	Rational Coâ€Design of Polymer Dielectrics for Energy Storage. Advanced Materials, 2016, 28, 6277-6291.	11.1	149
9	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. Materials Today, 2018, 21, 785-796.	8.3	143
10	A polymer dataset for accelerated property prediction and design. Scientific Data, 2016, 3, 160012.	2.4	139
11	Dopants Promoting Ferroelectricity in Hafnia: Insights from a comprehensive Chemical Space Exploration. Chemistry of Materials, 2017, 29, 9102-9109.	3.2	139
12	Accelerated materials property predictions and design using motif-based fingerprints. Physical Review B, 2015, 92, .	1.1	136
13	Polymer informatics: Current status and critical next steps. Materials Science and Engineering Reports, 2021, 144, 100595.	14.8	117
14	A hybrid organic-inorganic perovskite dataset. Scientific Data, 2017, 4, 170057.	2.4	112
15	Machine-learning predictions of polymer properties with Polymer Genome. Journal of Applied Physics, 2020, 128, .	1.1	111
16	Stabilization of metastable phases in hafnia owing to surface energy effects. Applied Physics Letters, 2016, 108, .	1.5	108
17	Polymer design using genetic algorithm and machine learning. Computational Materials Science, 2021, 186, 110067.	1.4	105
18	Activating low-temperature diesel oxidation by single-atom Pt on TiO2 nanowire array. Nature Communications, 2020, 11, 1062.	5.8	90

#	Article	IF	Citations
19	Machine learning models for the lattice thermal conductivity prediction of inorganic materials. Computational Materials Science, 2019, 170, 109155.	1.4	84
20	Frequency-dependent dielectric constant prediction of polymers using machine learning. Npj Computational Materials, 2020, 6, .	3.5	75
21	Poly(dimethyltin glutarate) as a Prospective Material for High Dielectric Applications. Advanced Materials, 2015, 27, 346-351.	11.1	64
22	Interlayer Interactions in van der Waals Heterostructures: Electron and Phonon Properties. ACS Applied Materials & Interfaces, 2016, 8, 6286-6292.	4.0	63
23	Role of Oxygen Vacancy Defects in the Electrocatalytic Activity of Substoichiometric Molybdenum Oxide. Journal of Physical Chemistry C, 2018, 122, 18212-18222.	1.5	63
24	Charge injection barriers at metal/polyethylene interfaces. Journal of Materials Science, 2016, 51, 506-512.	1.7	56
25	Rational Design of Organotin Polyesters. Macromolecules, 2015, 48, 2422-2428.	2.2	54
26	Electronic Structure of Polyethylene: Role of Chemical, Morphological and Interfacial Complexity. Scientific Reports, 2017, 7, 6128.	1.6	53
27	A multi-fidelity information-fusion approach to machine learn and predict polymer bandgap. Computational Materials Science, 2020, 172, 109286.	1.4	49
28	Mining Materials Design Rules from Data: The Example of Polymer Dielectrics. Chemistry of Materials, 2017, 29, 9001-9010.	3.2	48
29	Novel Structural Motifs in Low Energy Phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiAlH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 205505.	2.9	43
30	Polymers for Extreme Conditions Designed Using Syntax-Directed Variational Autoencoders. Chemistry of Materials, 2020, 32, 10489-10500.	3.2	43
31	Polymer informatics with multi-task learning. Patterns, 2021, 2, 100238.	3.1	43
32	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	2.9	38
33	Polyelectrolyte-Assisted Oxygen Vacancies: A New Route to Defect Engineering in Molybdenum Oxide. Langmuir, 2018, 34, 6296-6306.	1.6	35
34	General Atomic Neighborhood Fingerprint for Machine Learning-Based Methods. Journal of Physical Chemistry C, 2019, 123, 15859-15866.	1.5	33
35	Layered structures of organic/inorganic hybrid halide perovskites. Physical Review B, 2016, 93, .	1.1	31
36	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29

#	Article	IF	Citations
37	Effect of Incorporating Aromatic and Chiral Groups on the Dielectric Properties of Poly(dimethyltin) Tj ETQq1 1 0.784314 rgBT /Overlock	2.0	29
38	Modulating Polymerization Thermodynamics of Thiolactones Through Substituent and Heteroatom Incorporation. ACS Macro Letters, 2022, 11, 895-901.	2.3	28
39	Low-energy structures of zinc borohydride Zn(BH<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 677 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	27
40	Roughness-induced piezoelectric scattering in lattice-mismatched semiconductor quantum wells. Physical Review B, 2003, 68, .	1.1	26
41	Tunable Spin-Dependent Properties of Zigzag Silicene Nanoribbons. Physical Review Applied, 2014, 1, .	1.5	26
42	High-pressure phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Mg</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> first principles. Physical Review B, 2016, 93, .	1.1	26
43	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25
44	Block Copolymer-Assisted Solvothermal Synthesis of Hollow Bi₂MoO₆ Spheres Substituted with Samarium. Langmuir, 2016, 32, 10967-10976.	1.6	24
45	polyG2G: A Novel Machine Learning Algorithm Applied to the Generative Design of Polymer Dielectrics. Chemistry of Materials, 2021, 33, 7008-7016.	3.2	23
46	Random Piezoelectric Field in Real [001]-Oriented Strain-Relaxed Semiconductor Heterostructures. Physical Review Letters, 2002, 89, 077601.	2.9	21
47	Unraveling the luminescence signatures of chemical defects in polyethylene. Journal of Chemical Physics, 2015, 143, 124907.	1.2	21
48	Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers. ACS Applied Materials & Interfaces, 2020, 12, 37182-37187.	4.0	21
49	Iterative-Learning Strategy for the Development of Application-Specific Atomistic Force Fields. Journal of Physical Chemistry C, 2019, 123, 20715-20722.	1.5	20
50	Polymer Structure Prediction from First Principles. Journal of Physical Chemistry Letters, 2020, 11, 5823-5829.	2.1	20
51	Dielectric Polymers Tolerant to Electric Field and Temperature Extremes: Integration of Phenomenology, Informatics, and Experimental Validation. ACS Applied Materials & Interfaces, 2021, 13, 53416-53424.	4.0	20
52	Low-temperature mobility of holes inSiâˆ•SiGep-channel heterostructures. Physical Review B, 2004, 70, .	1.1	16
53	Theoretical prediction of low-density hexagonal ZnO hollow structures. Journal of Applied Physics, 2016, 120, .	1.1	15
54	Strong Rashbaâ€Dresselhaus Effect in Nonchiral 2D Ruddlesdenâ€Popper Perovskites. Advanced Optical Materials, 2022, 10, 2101232.	3.6	14

#	Article	IF	Citations
55	Exploring PtSO4 and PdSO4 phases: an evolutionary algorithm based investigation. Physical Chemistry Chemical Physics, 2015, 17, 18146-18151.	1.3	13
56	Pressure-stabilized binary compounds of magnesium and silicon. Physical Review Materials, 2018, 2, .	0.9	13
57	An Efficient Deep Learning Scheme To Predict the Electronic Structure of Materials and Molecules: The Example of Graphene-Derived Allotropes. Journal of Physical Chemistry A, 2020, 124, 9496-9502.	1.1	12
58	Novel high voltage polymer insulators using computational and data-driven techniques. Journal of Chemical Physics, 2021, 154, 174906.	1.2	12
59	Toward Recyclable Polymers: Ring-Opening Polymerization Enthalpy from First-Principles. Journal of Physical Chemistry Letters, 2022, 13, 4778-4785.	2.1	12
60	Atomistic mechanisms for chemical defects formation in polyethylene. Journal of Chemical Physics, 2018, 149, 234902.	1.2	11
61	Strain fluctuations in a real [001]-oriented zinc-blende-structure surface quantum well. Physical Review B, 2003, 68, .	1.1	10
62	Valence bond entanglement and fluctuations in random singlet phases. Physical Review B, 2011, 84, .	1.1	10
63	Computational predictions of zinc oxide hollow structures. Physica B: Condensed Matter, 2018, 532, 15-19.	1.3	9
64	Search for Ferroelectric Binary Oxides: Chemical and Structural Space Exploration Guided by Group Theory and Computations. Chemistry of Materials, 2020, 32, 3823-3832.	3.2	9
65	Modeling study on the properties of GaN/AlN core/shell nanowires by surface effect suppression. Physica Status Solidi (B): Basic Research, 2012, 249, 1241-1249.	0.7	8
66	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. Journal of Physical Chemistry Letters, 2019, 10, 3937-3943.	2.1	8
67	Monte Carlo simulations of interacting anyon chains. Computational Materials Science, 2010, 49, S395-S398.	1.4	7
68	Density functional theory based tight binding study on theoretical prediction of low-density nanoporous phases ZnO semiconductor materials. Journal of Physics: Conference Series, 2016, 726, 012022.	0.3	7
69	Compositional Effects and Electron Loneâ€pair Distortions in Doped Bournonites. ChemPhysChem, 2018, 19, 2635-2644.	1.0	7
70	High dielectric constant and high breakdown strength polyimide via tin complexation of the polyamide acid precursor. RSC Advances, 2022, 12, 9095-9100.	1.7	7
71	Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries. Journal of Chemical Theory and Computation, 2022, 18, 2737-2748.	2.3	7
72	Cage disorder and gas encapsulation as routes to tailor properties of inorganic clathrates. Acta Materialia, 2017, 131, 475-481.	3.8	6

#	Article	IF	Citations
73	Predicted Binary Compounds of Tin and Sulfur. Journal of Physical Chemistry C, 2018, 122, 17067-17072.	1.5	6
74	Lead-free hybrid organic-inorganic perovskites for solar cell applications. Journal of Chemical Physics, 2020, 152, 014104.	1.2	6
75	Sizeâ€induced structural transition in ZnO prismatic nanoparticles. Physica Status Solidi (B): Basic Research, 2012, 249, 535-543.	0.7	5
76	First-principles prediction for the stability of LiK(BH4)2. Physica Status Solidi (B): Basic Research, 2014, 251, 1539-1544.	0.7	5
77	Probabilistic deep learning approach for targeted hybrid organic-inorganic perovskites. Physical Review Materials, 2021, 5, .	0.9	5
78	Novel cage-like nanoporous ZnO polymorphs with cubic lattice frameworks. Materials Today Communications, 2020, 24, 101152.	0.9	4
79	Atomic configurations for materials research: A case study of some simple binary compounds. AIP Advances, 2021, 11, .	0.6	4
80	Impact of Surface on the <inline-formula> <tex-math notation="TeX">d^{0} </tex-math></inline-formula> Ferromagnetism of Lithium-Doped Zinc Oxide Nanowires. IEEE Transactions on Magnetics, 2014, 50, 1-7.	1.2	3
81	Characterizing magnesiumâ€“silicon binaries in Alâ€“Mgâ€“Si supersaturated solid solution by first-principles calculations. Journal of Science: Advanced Materials and Devices, 2016, 1, 527-530.	1.5	3
82	Thermal transport in phase-stabilized lithium zirconate phosphates. Applied Physics Letters, 2020, 117, 011903.	1.5	3
83	Structural, Electronic and Mechanical Properties of Few-Layer GaN Nanosheet: A First-Principle Study. Materials Transactions, 2020, 61, 1438-1444.	0.4	3
84	Diffusion thermopower of a p-type Si/Si1â€“xGex heterostructure at zero magnetic field. Physica Status Solidi (B): Basic Research, 2007, 244, 2100-2108.	0.7	2
85	Highly charged interface trap states in PbS1â^'x govern electro-thermal transport. APL Materials, 2019, 7, 071105.	2.2	2
86	Effect of impurity correlation in modulation-doped quantum wires. Physical Review B, 2001, 64, .	1.1	1
87	First-principles study of aluminum-polyethylene interfaces. , 2014, , .		1
88	Accelerating quantum molecular simulations. Nature Computational Science, 2022, 2, 292-293.	3.8	0