Tran Doan Huan

List of Publications by Year in Descending Order

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	High dielectric constant and high breakdown strength polyimide tin complexation of the polyamide acid precursor.. *RSC Advances*, **2022**, 12, 9095-9100	3.7	0
83	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**,	6.4	1
82	Polymer informatics: Current status and critical next steps. *Materials Science and Engineering Reports*, **2021**, 144, 100595	30.9	33
81	Polymer informatics with multi-task learning. *Patterns*, **2021**, 2, 100238	5.1	7
80	Atomic configurations for materials research: A case study of some simple binary compounds. *AIP Advances*, **2021**, 11, 045120	1.5	0
79	Novel high voltage polymer insulators using computational and data-driven techniques. *Journal of Chemical Physics*, **2021**, 154, 174906	3.9	3
78	Polymer design using genetic algorithm and machine learning. *Computational Materials Science*, **2021**, 186, 110067	3.2	43
77	Dielectric Polymers Tolerant to Electric Field and Temperature Extremes: Integration of Phenomenology, Informatics, and Experimental Validation. *ACS Applied Materials & Interfaces*, **2021**, 13, 53416-53424	9.5	5
76	polyG2G: A Novel Machine Learning Algorithm Applied to the Generative Design of Polymer Dielectrics. *Chemistry of Materials*, **2021**, 33, 7008-7016	9.6	4
75	Polymers for Extreme Conditions Designed Using Syntax-Directed Variational Autoencoders. *Chemistry of Materials*, **2020**, 32, 10489-10500	9.6	21
74	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	2.8	2
73	Frequency-dependent dielectric constant prediction of polymers using machine learning. *Npj Computational Materials*, **2020**, 6,	10.9	35
72	Novel cage-like nanoporous ZnO polymorphs with cubic lattice frameworks. *Materials Today Communications*, **2020**, 24, 101152	2.5	3
71	Thermal transport in phase-stabilized lithium zirconate phosphates. *Applied Physics Letters*, **2020**, 117, 011903	3.4	3
70	Polymer Structure Prediction from First Principles. *Journal of Physical Chemistry Letters*, **2020**, 11, 5823-5829	6.4	11
69	Activating low-temperature diesel oxidation by single-atom Pt on TiO nanowire array. *Nature Communications*, **2020**, 11, 1062	17.4	42
68	Lead-free hybrid organic-inorganic perovskites for solar cell applications. *Journal of Chemical Physics*, **2020**, 152, 014104	3.9	3

67	Search for Ferroelectric Binary Oxides: Chemical and Structural Space Exploration Guided by Group Theory and Computations. *Chemistry of Materials*, **2020**, 32, 3823-3832	9.6	3
66	Structural, Electronic and Mechanical Properties of Few-Layer GaN Nanosheet: A First-Principle Study. *Materials Transactions*, **2020**, 61, 1438-1444	1.3	0
65	Machine-learning predictions of polymer properties with Polymer Genome. *Journal of Applied Physics*, **2020**, 128, 171104	2.5	41
64	Computable Bulk and Interfacial Electronic Structure Features as Proxies for Dielectric Breakdown of Polymers. *ACS Applied Materials & Interfaces*, **2020**, 12, 37182-37187	9.5	11
63	A multi-fidelity information-fusion approach to machine learn and predict polymer bandgap. *Computational Materials Science*, **2020**, 172, 109286	3.2	27
62	General Atomic Neighborhood Fingerprint for Machine Learning-Based Methods. *Journal of Physical Chemistry C*, **2019**, 123, 15859-15866	3.8	23
61	Iterative-Learning Strategy for the Development of Application-Specific Atomistic Force Fields. *Journal of Physical Chemistry C*, **2019**, 123, 20715-20722	3.8	18
60	Machine learning models for the lattice thermal conductivity prediction of inorganic materials. *Computational Materials Science*, **2019**, 170, 109155	3.2	49
59	Highly charged interface trap states in PbS1⊠ govern electro-thermal transport. *APL Materials*, **2019**, 7, 071105	5.7	
58	Hot-Carrier Dynamics and Chemistry in Dielectric Polymers. *Journal of Physical Chemistry Letters*, **2019**, 10, 3937-3943	6.4	6
57	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. *Materials Today*, **2018**, 21, 785-796	21.8	99
56	Polyelectrolyte-Assisted Oxygen Vacancies: A New Route to Defect Engineering in Molybdenum Oxide. *Langmuir*, **2018**, 34, 6296-6306	4	26
55	Computational predictions of zinc oxide hollow structures. *Physica B: Condensed Matter*, **2018**, 532, 15-19	2.8	7
54	Compositional Effects and Electron Lone-pair Distortions in Doped Bournonites. *ChemPhysChem*, **2018**, 19, 2635-2644	3.2	5
53	Role of Oxygen Vacancy Defects in the Electrocatalytic Activity of Substoichiometric Molybdenum Oxide. *Journal of Physical Chemistry C*, **2018**, 122, 18212-18222	3.8	42
52	Polymer Genome: A Data-Powered Polymer Informatics Platform for Property Predictions. *Journal of Physical Chemistry C*, **2018**, 122, 17575-17585	3.8	156
51	Predicted Binary Compounds of Tin and Sulfur. *Journal of Physical Chemistry C*, **2018**, 122, 17067-17072	3.8	5
50	Pressure-stabilized binary compounds of magnesium and silicon. *Physical Review Materials*, **2018**, 2,	3.2	9

49	Atomistic mechanisms for chemical defects formation in polyethylene. *Journal of Chemical Physics*, **2018**, 149, 234902	3.9	10
48	Factors Favoring Ferroelectricity in Hafnia: A First-Principles Computational Study. *Journal of Physical Chemistry C*, **2017**, 121, 4139-4145	3.8	105
47	A hybrid organic-inorganic perovskite dataset. *Scientific Data*, **2017**, 4, 170057	8.2	73
46	Mining Materials Design Rules from Data: The Example of Polymer Dielectrics. *Chemistry of Materials*, **2017**, 29, 9001-9010	9.6	36
45	Dopants Promoting Ferroelectricity in Hafnia: Insights from a comprehensive Chemical Space Exploration. *Chemistry of Materials*, **2017**, 29, 9102-9109	9.6	87
44	A universal strategy for the creation of machine learning-based atomistic force fields. *Npj Computational Materials*, **2017**, 3,	10.9	155
43	Cage disorder and gas encapsulation as routes to tailor properties of inorganic clathrates. *Acta Materialia*, **2017**, 131, 475-481	8.4	5
42	Electronic Structure of Polyethylene: Role of Chemical, Morphological and Interfacial Complexity. *Scientific Reports*, **2017**, 7, 6128	4.9	34
41	High-pressure phases of Mg2Si from first principles. *Physical Review B*, **2016**, 93,	3.3	23
40	Layered structures of organic/inorganic hybrid halide perovskites. *Physical Review B*, **2016**, 93,	3.3	29
39	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	4
38	Machine Learning Strategy for Accelerated Design of Polymer Dielectrics. *Scientific Reports*, **2016**, 6, 20952	4.9	207
37	Rational Co-Design of Polymer Dielectrics for Energy Storage. *Advanced Materials*, **2016**, 28, 6277-91	24	118
36	Interlayer Interactions in van der Waals Heterostructures: Electron and Phonon Properties. *ACS Applied Materials & Interfaces*, **2016**, 8, 6286-92	9.5	53
35	Charge injection barriers at metal/polyethylene interfaces. *Journal of Materials Science*, **2016**, 51, 506-512	4.3	42
34	Mesoporous MoO3− Material as an Efficient Electrocatalyst for Hydrogen Evolution Reactions. *Advanced Energy Materials*, **2016**, 6, 1600528	21.8	262
33	Theoretical prediction of low-density hexagonal ZnO hollow structures. *Journal of Applied Physics*, **2016**, 120, 142105	2.5	11
32	Stabilization of metastable phases in hafnia owing to surface energy effects. *Applied Physics Letters* , **2016**, 108, 172902	3.4	74

31	A polymer dataset for accelerated property prediction and design. *Scientific Data*, **2016**, 3, 160012	8.2	100
30	Advanced polymeric dielectrics for high energy density applications. *Progress in Materials Science*, **2016**, 83, 236-269	42.2	193
29	Characterizing magnesium□silicon binaries in Al□Mg□Si supersaturated solid solution by first-principles calculations. *Journal of Science: Advanced Materials and Devices*, **2016**, 1, 527-530	4.2	3
28	Block Copolymer-Assisted Solvothermal Synthesis of Hollow BiMoO Spheres Substituted with Samarium. *Langmuir*, **2016**, 32, 10967-10976	4	21
27	Rational Design of Organotin Polyesters. *Macromolecules*, **2015**, 48, 2422-2428	5.5	47
26	Exploring PtSO4 and PdSO4 phases: an evolutionary algorithm based investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 18146-51	3.6	13
25	Poly(dimethyltin glutarate) as a prospective material for high dielectric applications. *Advanced Materials*, **2015**, 27, 346-51	24	52
24	Unraveling the luminescence signatures of chemical defects in polyethylene. *Journal of Chemical Physics*, **2015**, 143, 124907	3.9	21
23	Accelerated materials property predictions and design using motif-based fingerprints. *Physical Review B*, **2015**, 92,	3.3	111
22	Impact of Surface on the d^{0} Ferromagnetism of Lithium-Doped Zinc Oxide Nanowires. *IEEE Transactions on Magnetics*, **2014**, 50, 1-7	2	2
21	Tunable Spin-Dependent Properties of Zigzag Silicene Nanoribbons. *Physical Review Applied*, **2014**, 1,	4.3	26
20	First-principles prediction for the stability of LiK(. *Physica Status Solidi (B): Basic Research*, **2014**, 251, 1539-1544	1.3	4
19	Effect of incorporating aromatic and chiral groups on the dielectric properties of poly(dimethyltin esters). *Macromolecular Rapid Communications*, **2014**, 35, 2082-8	4.8	26
18	Pathways towards ferroelectricity in hafnia. *Physical Review B*, **2014**, 90,	3.3	230
17	First-principles predicted low-energy structures of NaSc(BH4)4. *Journal of Chemical Physics*, **2014**, 140, 124708	3.9	17
16	Thermodynamic stability of alkali-metal□zinc double-cation borohydrides at low temperatures. *Physical Review B*, **2013**, 88,	3.3	27
15	Low-energy polymeric phases of alanates. *Physical Review Letters*, **2013**, 110, 135502	7.4	33
14	Low-energy structures of zinc borohydride Zn(BH4)2. *Physical Review B*, **2012**, 86,	3.3	26

13	Size-induced structural transition in ZnO prismatic nanoparticles. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 535-543	1.3	5
12	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	1.3	7
11	Novel structural motifs in low energy phases of LiAlH4. *Physical Review Letters*, **2012**, 108, 205505	7.4	42
10	Valence bond entanglement and fluctuations in random singlet phases. *Physical Review B*, **2011**, 84,	3.3	9
9	Monte Carlo simulations of interacting anyon chains. *Computational Materials Science*, **2010**, 49, S395-S398	1.2	5
8	Diffusion thermopower of a p-type Si/Si1 Gex heterostructure at zero magnetic field. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 2100-2108	1.3	1
7	Low-temperature mobility of holes in SiSiGe p-channel heterostructures. *Physical Review B*, **2004**, 70,	3.3	16
6	Roughness-induced piezoelectric scattering in lattice-mismatched semiconductor quantum wells. *Physical Review B*, **2003**, 68,	3.3	19
5	Strain fluctuations in a real [001]-oriented zinc-blende-structure surface quantum well. *Physical Review B*, **2003**, 68,	3.3	10
4	Random piezoelectric field in real [001]-oriented strain-relaxed semiconductor heterostructures. *Physical Review Letters*, **2002**, 89, 077601	7.4	19
3	Effect of impurity correlation in modulation-doped quantum wires. *Physical Review B*, **2001**, 64,	3.3	1
2	Strong Rashba-Dresselhaus Effect in Nonchiral 2D Ruddlesden-Popper Perovskites. *Advanced Optical Materials*,2101232	8.1	1
1	Toward Recyclable Polymers: Ring-Opening Polymerization Enthalpy from First-Principles. *Journal of Physical Chemistry Letters*,4778-4785	6.4	1