Ghanshyam Pilania

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9316953/publications.pdf

Version: 2024-02-01

93 papers	5,836 citations	117625 34 h-index	74163 75 g-index
96 all docs	96 docs citations	96 times ranked	5600 citing authors

#	Article	IF	Citations
1	Machine learning in materials informatics: recent applications and prospects. Npj Computational Materials, 2017, 3, .	8.7	1,013
2	Accelerating materials property predictions using machine learning. Scientific Reports, 2013, 3, 2810.	3.3	574
3	Machine learning bandgaps of double perovskites. Scientific Reports, 2016, 6, 19375.	3.3	354
4	Machine Learning Strategy for Accelerated Design of Polymer Dielectrics. Scientific Reports, 2016, 6, 20952.	3.3	279
5	Rational design of all organic polymer dielectrics. Nature Communications, 2014, 5, 4845.	12.8	259
6	Multi-fidelity machine learning models for accurate bandgap predictions of solids. Computational Materials Science, 2017, 129, 156-163.	3.0	235
7	From Organized High-Throughput Data to Phenomenological Theory using Machine Learning: The Example of Dielectric Breakdown. Chemistry of Materials, 2016, 28, 1304-1311.	6.7	184
8	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	8.7	181
9	Machine Learning Assisted Predictions of Intrinsic Dielectric Breakdown Strength of ABX₃ Perovskites. Journal of Physical Chemistry C, 2016, 120, 14575-14580.	3.1	147
10	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. Materials Today, 2018, 21, 785-796.	14.2	143
11	A polymer dataset for accelerated property prediction and design. Scientific Data, 2016, 3, 160012.	5.3	139
12	Finding New Perovskite Halides via Machine Learning. Frontiers in Materials, 2016, 3, .	2.4	138
13	Polymer informatics: Current status and critical next steps. Materials Science and Engineering Reports, 2021, 144, 100595.	31.8	117
14	Computational strategies for polymer dielectrics design. Polymer, 2014, 55, 979-988.	3.8	116
15	Machine learning in materials science: From explainable predictions to autonomous design. Computational Materials Science, 2021, 193, 110360.	3.0	103
16	Machine-Learning-Based Predictive Modeling of Glass Transition Temperatures: A Case of Polyhydroxyalkanoate Homopolymers and Copolymers. Journal of Chemical Information and Modeling, 2019, 59, 5013-5025.	5.4	85
17	Developing an interatomic potential for martensitic phase transformations in zirconium by machine learning. Npj Computational Materials, 2018, 4, .	8.7	79
18	Revisiting the Al/Al2O3 Interface: Coherent Interfaces and Misfit Accommodation. Scientific Reports, 2014, 4, 4485.	3.3	78

#	Article	IF	Citations
19	Structure classification and melting temperature prediction in octet AB solids via machine learning. Physical Review B, 2015, 91, .	3.2	65
20	A Machine Learning Approach for the Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Chemistry of Materials, 2021, 33, 845-858.	6.7	64
21	Ab initiostudy of ferroelectricity inBaTiO3nanowires. Physical Review B, 2009, 80, .	3.2	63
22	How Critical Are the van der Waals Interactions in Polymer Crystals?. Journal of Physical Chemistry A, 2012, 116, 9347-9352.	2.5	63
23	Classification ofABO₃perovskite solids: a machine learning study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 507-513.	1.1	56
24	Multifidelity Information Fusion with Machine Learning: A Case Study of Dopant Formation Energies in Hafnia. ACS Applied Materials & Interfaces, 2019, 11, 24906-24918.	8.0	49
25	KBaTeBiO₆: A Lead-Free, Inorganic Double-Perovskite Semiconductor for Photovoltaic Applications. Chemistry of Materials, 2019, 31, 4769-4778.	6.7	46
26	Prediction of structure and cation ordering in an ordered normal-inverse double spinel. Communications Materials, 2020, 1, .	6.9	46
27	Critical assessment of regression-based machine learning methods for polymer dielectrics. Computational Materials Science, 2016, 125, 123-135.	3.0	45
28	Comprehensive examination of dopants and defects in BaTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>from first principles. Physical Review B, 2013, 87, .	3.2	43
29	Enhanced Polymeric Dielectrics through Incorporation of Hydroxyl Groups. Macromolecules, 2014, 47, 1122-1129.	4.8	43
30	Machine learning in nuclear materials research. Current Opinion in Solid State and Materials Science, 2022, 26, 100975.	11.5	42
31	Machine learning for materials design and discovery. Journal of Applied Physics, 2021, 129, .	2.5	41
32	Termination chemistry-driven dislocation structure at SrTiO3/MgO heterointerfaces. Nature Communications, 2014, 5, 5043.	12.8	39
33	Complex polarization ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>A first-principles computational study. Physical Review B, 2010, 82, .	3.2	37
34	Adsorption of atomic oxygen on cubic PbTiO3 and LaMnO3 (001) surfaces: A density functional theory study. Surface Science, 2010, 604, 1889-1893.	1.9	36
35	Electronic, magnetic, optical and elastic properties of Fe2YAl (Y=Ti, V and Cr) using first principles methods. Journal of Magnetism and Magnetic Materials, 2013, 339, 142-150.	2.3	36
36	Machine learning elastic constants of multi-component alloys. Computational Materials Science, 2021, 198, 110671.	3.0	36

#	Article	IF	Citations
37	High-throughput investigation of the formation of double spinels. Journal of Materials Chemistry A, 2020, 8, 25756-25767.	10.3	36
38	New Group IV Chemical Motifs for Improved Dielectric Permittivity of Polyethylene. Journal of Chemical Information and Modeling, 2013, 53, 879-886.	5.4	34
39	Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583.	6.7	33
40	Effect of Cation Ordering on Oxygen Vacancy Diffusion Pathways in Double Perovskites. Chemistry of Materials, 2015, 27, 5020-5026.	6.7	32
41	Dielectric properties of carbon-, silicon-, and germanium-based polymers: A first-principles study. Physical Review B, 2013, 87, .	3.2	31
42	Multi-objective optimization techniques to design the Pareto front of organic dielectric polymers. Computational Materials Science, 2016, 125, 92-99.	3.0	31
43	Physics-informed machine learning for inorganic scintillator discovery. Journal of Chemical Physics, 2018, 148, 241729.	3.0	28
44	Machine learning properties of binary wurtzite superlattices. Journal of Materials Science, 2018, 53, 6652-6664.	3.7	24
45	Dielectric permittivity of ultrathin PbTiO3 nanowires from first principles. Journal of Materials Science, 2012, 47, 7580-7586.	3.7	23
46	Distortion-stabilized ordered structures in A2BBâ€™O7 mixed pyrochlores. Npj Computational Materials, 2019, 5, .	8.7	23
47	Anion order in oxysulfide perovskites: origins and implications. Npj Computational Materials, 2020, 6, .	8.7	22
48	Establishing the LaMnO₃ Surface Phase Diagram in an Oxygen Environment: An ab Initio Kinetic Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2012, 116, 26349-26357.	3.1	21
49	Machine learning substitutional defect formation energies in ABO3 perovskites. Journal of Applied Physics, 2020, 128, .	2.5	21
50	Roads less traveled: Nitrogen reduction reaction catalyst design strategies for improved selectivity. Current Opinion in Electrochemistry, 2021, 28, 100723.	4.8	20
51	Ab initio study of antiferroelectric PbZrO3 (001) surfaces. Journal of Materials Science, 2009, 44, 5249-5255.	3.7	19
52	Ferromagnetism in IV main group element (C) and transition metal (Mn) doped MgO: A density functional perspective. AIP Advances, 2011, 1, 032129.	1.3	19
53	First principles investigations of structural, electronic, elastic, and dielectric properties of KMgF3. Journal of Materials Science, 2013, 48, 7635-7641.	3.7	19
54	Semicoherent oxide heterointerfaces: Structure, properties, and implications. APL Materials, 2019, 7, .	5.1	19

#	Article	IF	Citations
55	Molecular dynamics simulations for glass transition temperature predictions of polyhydroxyalkanoate biopolymers. Physical Chemistry Chemical Physics, 2020, 22, 17880-17889.	2.8	19
56	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. ACS Applied Materials & Interfaces, 2020, 12, 46296-46305.	8.0	19
57	A Perspective on Materials Informatics: State-of-the-Art and Challenges. Springer Series in Materials Science, 2016, , 3-12.	0.6	18
58	Oxygen Adsorption on CdSe Surfaces: Case Study of Asymmetric Anisotropic Growth through ab Initio Computations. Journal of Physical Chemistry C, 2009, 113, 1863-1871.	3.1	15
59	Role of Multiple Charge States of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Ce</mml:mi></mml:math> in the Scintillation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi mathvariant="italic">AB</mml:mi><mml:msub><mml:mrow><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:math>	3.8	15
60	Machine Learning for Melting Temperature Predictions and Design in Polyhydroxyalkanoate-Based Biopolymers. Journal of Physical Chemistry B, 2022, 126, 934-945.	2.6	15
61	Electronic, phonon, and dielectric properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">RbHgF</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> perovskite and hybrid improper ferroelectricity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mo>(</mml:mo><mml:mtext>Na</mml:mtext><mml:mo>,</mml:mo><mml:mi mathvariant="normal">Hg</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvaria	3.2	14
62	Classification of octet AB-type binary compounds using dynamical charges: A materials informatics perspective. Scientific Reports, 2015, 5, 17504.	3.3	14
63	Oxygen-Assisted Unidirectional Growth of CdSe Nanorods Using a Low-Temperature Redox Process. Nano Letters, 2010, 10, 680-685.	9.1	13
64	A Deep Neural Network for Accurate and Robust Prediction of the Glass Transition Temperature of Polyhydroxyalkanoate Homo- and Copolymers. Materials, 2020, 13, 5701.	2.9	12
65	Dielectric permittivity enhancement in hydroxyl functionalized polyolefins via cooperative interactions with water. Applied Physics Letters, 2013, 102, 152901.	3.3	11
66	Composition and Configuration Dependence of Glass-Transition Temperature in Binary Copolymers and Blends of Polyhydroxyalkanoate Biopolymers. Macromolecules, 2021, 54, 5618-5628.	4.8	11
67	First-principles identification of novel double perovskites for water-splitting applications. Journal of Materials Science, 2017, 52, 8518-8525.	3.7	10
68	Data-enabled structureâ€“property mappings for lanthanide-activated inorganic scintillators. Journal of Materials Science, 2019, 54, 8361-8380.	3.7	9
69	A comprehensive computational study of adatom diffusion on the aluminum (1â€¯0â€¯0) surface. Computational Materials Science, 2019, 158, 353-358.	3.0	9
70	The effect of aromatic and sulfur compounds on partial discharge characteristics of hexadecane. IEEE Transactions on Dielectrics and Electrical Insulation, 2013, 20, 801-813.	2.9	8
71	Cation ordering and effect of biaxial strain in double perovskite CsRbCaZnCl6. Journal of Applied Physics, 2015, 117, .	2.5	8
72	Accurately predicting optical properties of rare-earth, aluminate scintillators: influence of electronâ€“hole correlation. Journal of Materials Chemistry C, 2021, 9, 7292-7301.	5.5	8

#	Article	IF	Citations
73	A first-principles investigation of nitrogen reduction to ammonia on zirconium nitride and oxynitride surfaces. Journal of Materials Science, 2022, 57, 10213-10224.	3.7	8
74	Predicting the Mechanical Response of Polyhydroxyalkanoate Biopolymers Using Molecular Dynamics Simulations. Polymers, 2022, 14, 345.	4.5	7
75	Data-Based Methods for Materials Design and Discovery: Basic Ideas and General Methods. Synthesis Lectures on Materials and Optics, 2020, 1, 1-188.	0.2	6
76	Modeling Disorder in Pyrochlores and Other Anion-Deficient Fluorite Structural Derivative Oxides. Frontiers in Chemistry, 2021, 9, 712543.	3.6	6
77	Perovskite oxynitrides as tunable materials for electrocatalytic nitrogen reduction to ammonia. Trends in Chemistry, 2021, 3, 694-696.	8.5	6
78	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	3.7	6
79	First principles study of the interface between silicone and undoped/doped BaTiO3. Journal of Applied Physics, 2013, 113, .	2.5	5
80	The impact of chemical order on defect transport in mixed pyrochlores. Physical Chemistry Chemical Physics, 2019, 21, 5956-5965.	2.8	5
81	Effect of lattice strain on magnetism in epitaxial YCrO₃ films. Materials Research Letters, 2022, 10, 29-35.	8.7	5
82	Computational screening of organic polymer dielectrics for novel accelerator technologies. Scientific Reports, 2018, 8, 9258.	3.3	4
83	Role of Symmetry, Geometry, and Termination Chemistry on Misfit Dislocation Patterns at Semicoherent Heterointerfaces. Matter, 2020, 2, 1324-1337.	10.0	4
84	Tuning magnetic and optical properties through strain in epitaxial LaCrO3 thin films. Applied Physics Letters, 2021, 119, .	3.3	4
85	The effect of oxidative and paper degradation impurities on partial discharge characteristics of hexadecane. IEEE Transactions on Dielectrics and Electrical Insulation, 2013, 20, 1669-1682.	2.9	3
86	Inversion, chemical complexity, and interstitial transport in spinels. Journal of the American Ceramic Society, 2021, 104, 2313-2324.	3.8	2
87	Strong Purcell enhancement at telecom wavelengths afforded by spinel Fe3O4 nanocrystals with size-tunable plasmonic properties. Nanoscale Horizons, 2021, , .	8.0	2
88	First principles approach to ionicity of fragments. Chemical Physics, 2015, 448, 26-33.	1.9	1
89	Strong Zeeman splitting in orbital-hybridized valleytronic interfaces. Journal of Materials Science, 0, , 1.	3.7	1
90	Defect thermodynamics in spinel oxides leading to plasmonic behavior. Journal of Physics and Chemistry of Solids, 2022, 168, 110822.	4.0	1

#	Article	IF	Citations
91	Thermodynamics of Oxygen Chemistry on PbTiO3 and LaMnO3 (001) Surfaces. Materials Research Society Symposia Proceedings, 2011, 1309, 151.	0.1	0
92	Communication: Fragment-based Hamiltonian model of electronic charge-excitation gaps and gap closure. Journal of Chemical Physics, 2015, 143, 181104.	3.0	0
93	Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. Journal of Materials Science, 2021, 56, 15812-15823.	3.7	0