Ghanshyam Pilania

List of Publications by Year
in descending order

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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	Predicting the Mechanical Response of Polyhydroxyalkanoate Biopolymers Using Molecular Dynamics Simulations. Polymers, 2022, 14, 345.	4.5	7
2	Effect of lattice strain on magnetism in epitaxial YCrO₃ films. Materials Research Letters, 2022, 10, 29-35.	8.7	5
3	Machine Learning for Melting Temperature Predictions and Design in Polyhydroxyalkanoate-Based Biopolymers. Journal of Physical Chemistry B, 2022, 126, 934-945.	2.6	15
4	Machine learning in nuclear materials research. Current Opinion in Solid State and Materials Science, 2022, 26, 100975.	11.5	42
5	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
6	Defect thermodynamics in spinel oxides leading to plasmonic behavior. Journal of Physics and Chemistry of Solids, 2022, 168, 110822.	4.0	1
7	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	3.7	6
8	Inversion, chemical complexity, and interstitial transport in spinels. Journal of the American Ceramic Society, 2021, 104, 2313-2324.	3.8	2
9	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
10	Machine learning for materials design and discovery. Journal of Applied Physics, 2021, 129, .	2.5	41
11	Polymer informatics: Current status and critical next steps. Materials Science and Engineering Reports, 2021, 144, 100595.	31.8	117
12	Composition and Configuration Dependence of Glass-Transition Temperature in Binary Copolymers and Blends of Polyhydroxyalkanoate Biopolymers. Macromolecules, 2021, 54, 5618-5628.	4.8	11
13	Machine learning in materials science: From explainable predictions to autonomous design. Computational Materials Science, 2021, 193, 110360.	3.0	103
14	Barriers to carriers: faults and recombination in non-stoichiometric perovskite scintillators. Journal of Materials Science, 2021, 56, 15812-15823.	3.7	0
15	Modeling Disorder in Pyrochlores and Other Anion-Deficient Fluorite Structural Derivative Oxides. Frontiers in Chemistry, 2021, 9, 712543.	3.6	6
16	Roads less traveled: Nitrogen reduction reaction catalyst design strategies for improved selectivity. Current Opinion in Electrochemistry, 2021, 28, 100723.	4.8	20
17	Tuning magnetic and optical properties through strain in epitaxial LaCrO3 thin films. Applied Physics Letters, 2021, 119, .	3.3	4
18	Perovskite oxynitrides as tunable materials for electrocatalytic nitrogen reduction to ammonia. Trends in Chemistry, 2021, 3, 694-696.	8.5	6

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19	Machine learning elastic constants of multi-component alloys. Computational Materials Science, 2021, 198, 110671.	3.0	36
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	Strong Purcell enhancement at telecom wavelengths afforded by spinel Fe3O4 nanocrystals with size-tunable plasmonic properties. Nanoscale Horizons, 2021, , .	8.0	2
22	Role of Symmetry, Geometry, and Termination Chemistry on Misfit Dislocation Patterns at Semicoherent Heterointerfaces. Matter, 2020, 2, 1324-1337.	10.0	4
23	Machine learning substitutional defect formation energies in ABO3 perovskites. Journal of Applied Physics, 2020, 128, .	2.5	21
24	Molecular dynamics simulations for glass transition temperature predictions of polyhydroxyalkanoate biopolymers. Physical Chemistry Chemical Physics, 2020, 22, 17880-17889.	2.8	19
25	The joint automated repository for various integrated simulations (JARVIS) for data-driven materials design. Npj Computational Materials, 2020, 6, .	8.7	181
26	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. ACS Applied Materials & Interfaces, 2020, 12, 46296-46305.	8.0	19
27	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
28	Prediction of structure and cation ordering in an ordered normal-inverse double spinel. Communications Materials, 2020, 1, .	6.9	46
29	Anion order in oxysulfide perovskites: origins and implications. Npj Computational Materials, 2020, 6, .	8.7	22
30	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
31	High-throughput investigation of the formation of double spinels. Journal of Materials Chemistry A, 2020, 8, 25756-25767.	10.3	36
32	Semicoherent oxide heterointerfaces: Structure, properties, and implications. APL Materials, 2019, 7, .	5.1	19
33	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
34	KBaTeBiO₆: A Lead-Free, Inorganic Double-Perovskite Semiconductor for Photovoltaic Applications. Chemistry of Materials, 2019, 31, 4769-4778.	6.7	46
35	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
36	Data-enabled structureâ€“property mappings for lanthanide-activated inorganic scintillators. Journal of Materials Science, 2019, 54, 8361-8380.	3.7	9

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37	The impact of chemical order on defect transport in mixed pyrochlores. Physical Chemistry Chemical Physics, 2019, 21, 5956-5965.	2.8	5
38	Distortion-stabilized ordered structures in A2BBâ€™O7 mixed pyrochlores. Npj Computational Materials, 2019, 5, .	8.7	23
39	A comprehensive computational study of adatom diffusion on the aluminum (1â€¯0â€¯0) surface. Computational Materials Science, 2019, 158, 353-358.	3.0	9
40	Machine learning properties of binary wurtzite superlattices. Journal of Materials Science, 2018, 53, 6652-6664.	3.7	24
41	Scoping the polymer genome: A roadmap for rational polymer dielectrics design and beyond. Materials Today, 2018, 21, 785-796.	14.2	143
42	Physics-informed machine learning for inorganic scintillator discovery. Journal of Chemical Physics, 2018, 148, 241729.	3.0	28
43	Developing an interatomic potential for martensitic phase transformations in zirconium by machine learning. Npj Computational Materials, 2018, 4, .	8.7	79
44	Computational screening of organic polymer dielectrics for novel accelerator technologies. Scientific Reports, 2018, 8, 9258.	3.3	4
45	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
46	Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583.	6.7	33
47	First-principles identification of novel double perovskites for water-splitting applications. Journal of Materials Science, 2017, 52, 8518-8525.	3.7	10
48	Multi-fidelity machine learning models for accurate bandgap predictions of solids. Computational Materials Science, 2017, 129, 156-163.	3.0	235
49	Machine learning in materials informatics: recent applications and prospects. Npj Computational Materials, 2017, 3, .	8.7	1,013
50	Finding New Perovskite Halides via Machine Learning. Frontiers in Materials, 2016, 3, .	2.4	138
51	A polymer dataset for accelerated property prediction and design. Scientific Data, 2016, 3, 160012.	5.3	139
52	Multi-objective optimization techniques to design the Pareto front of organic dielectric polymers. Computational Materials Science, 2016, 125, 92-99.	3.0	31
53	Critical assessment of regression-based machine learning methods for polymer dielectrics. Computational Materials Science, 2016, 125, 123-135.	3.0	45
54	Machine learning bandgaps of double perovskites. Scientific Reports, 2016, 6, 19375.	3.3	354

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55	Machine Learning Strategy for Accelerated Design of Polymer Dielectrics. Scientific Reports, 2016, 6, 20952.	3.3	279
56	Machine Learning Assisted Predictions of Intrinsic Dielectric Breakdown Strength of ABX₃ Perovskites. Journal of Physical Chemistry C, 2016, 120, 14575-14580.	3.1	147
57	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
58	A Perspective on Materials Informatics: State-of-the-Art and Challenges. Springer Series in Materials Science, 2016, , 3-12.	0.6	18
59	Structure classification and melting temperature prediction in octet AB solids via machine learning. Physical Review B, 2015, 91, .	3.2	65
60	Communication: Fragment-based Hamiltonian model of electronic charge-excitation gaps and gap closure. Journal of Chemical Physics, 2015, 143, 181104.	3.0	0
61	Classification of octet AB-type binary compounds using dynamical charges: A materials informatics perspective. Scientific Reports, 2015, 5, 17504.	3.3	14
62	First principles approach to ionicity of fragments. Chemical Physics, 2015, 448, 26-33.	1.9	1
63	Effect of Cation Ordering on Oxygen Vacancy Diffusion Pathways in Double Perovskites. Chemistry of Materials, 2015, 27, 5020-5026.	6.7	32
64	Classification ofABO₃perovskite solids: a machine learning study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 507-513.	1.1	56
65	Cation ordering and effect of biaxial strain in double perovskite CsRbCaZnCl6. Journal of Applied Physics, 2015, 117, .	2.5	8
66	Computational strategies for polymer dielectrics design. Polymer, 2014, 55, 979-988.	3.8	116
67	Enhanced Polymeric Dielectrics through Incorporation of Hydroxyl Groups. Macromolecules, 2014, 47, 1122-1129.	4.8	43
68	Termination chemistry-driven dislocation structure at SrTiO3/MgO heterointerfaces. Nature Communications, 2014, 5, 5043.	12.8	39
69	Rational design of all organic polymer dielectrics. Nature Communications, 2014, 5, 4845.	12.8	259
70	Electronic structure and biaxial strain in<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
71	Revisiting the Al/Al2O3 Interface: Coherent Interfaces and Misfit Accommodation. Scientific Reports, 2014, 4, 4485.	3.3	78
72	First principles investigations of structural, electronic, elastic, and dielectric properties of KMgF3. Journal of Materials Science, 2013, 48, 7635-7641.	3.7	19

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73	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
74	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
75	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
76	New Group IV Chemical Motifs for Improved Dielectric Permittivity of Polyethylene. Journal of Chemical Information and Modeling, 2013, 53, 879-886.	5.4	34
77	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
78	Dielectric properties of carbon-, silicon-, and germanium-based polymers: A first-principles study. Physical Review B, 2013, 87, .	3.2	31
79	First principles study of the interface between silicone and undoped/doped BaTiO3. Journal of Applied Physics, 2013, 113, .	2.5	5
80	Dielectric permittivity enhancement in hydroxyl functionalized polyolefins via cooperative interactions with water. Applied Physics Letters, 2013, 102, 152901.	3.3	11
81	Accelerating materials property predictions using machine learning. Scientific Reports, 2013, 3, 2810.	3.3	574
82	Dielectric permittivity of ultrathin PbTiO3 nanowires from first principles. Journal of Materials Science, 2012, 47, 7580-7586.	3.7	23
83	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
84	How Critical Are the van der Waals Interactions in Polymer Crystals?. Journal of Physical Chemistry A, 2012, 116, 9347-9352.	2.5	63
85	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
86	Thermodynamics of Oxygen Chemistry on PbTiO3 and LaMnO3 (001) Surfaces. Materials Research Society Symposia Proceedings, 2011, 1309, 151.	0.1	0
87	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
88	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
89	Oxygen-Assisted Unidirectional Growth of CdSe Nanorods Using a Low-Temperature Redox Process. Nano Letters, 2010, 10, 680-685.	9.1	13
90	Ab initio study of antiferroelectric PbZrO3 (001) surfaces. Journal of Materials Science, 2009, 44, 5249-5255.	3.7	19

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91	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
92	Ab initiostudy of ferroelectricity inBaTiO3nanowires. Physical Review B, 2009, 80, .	3.2	63
93	Strong Zeeman splitting in orbital-hybridized valleytronic interfaces. Journal of Materials Science, 0, , 1.	3.7	1