Umesh V Waghmare

List of Publications by Year
in descending order

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85 papers	6,462 citations	87888 38 h-index	64796 79 g-index
87 all docs	87 docs citations	87 times ranked	7962 citing authors

#	Article	IF	Citations
1	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	13.6	698
2	Synthesis, Structure, and Properties of Boronâ€•and Nitrogenâ€Doped Graphene. Advanced Materials, 2009, 21, 4726-4730.	21.0	569
3	Mg Alloying in SnTe Facilitates Valence Band Convergence and Optimizes Thermoelectric Properties. Chemistry of Materials, 2015, 27, 581-587.	6.7	390
4	Ab initio statistical mechanics of the ferroelectric phase transition inPbTiO3. Physical Review B, 1997, 55, 6161-6173.	3.2	308
5	Enhanced atomic ordering leads to high thermoelectric performance in AgSbTe ₂. Science, 2021, 371, 722-727.	12.6	306
6	First-principles indicators of metallicity and cation off-centricity in the IV-VI rocksalt chalcogenides of divalent Ge, Sn, and Pb. Physical Review B, 2003, 67, .	3.2	299
7	Scale-free ferroelectricity induced by flat phonon bands in HfO ₂. Science, 2020, 369, 1343-1347.	12.6	231
8	High Power Factor and Enhanced Thermoelectric Performance of SnTe-AgInTe₂: Synergistic Effect of Resonance Level and Valence Band Convergence. Journal of the American Chemical Society, 2016, 138, 13068-13075.	13.7	214
9	BiferroicYCrO3. Physical Review B, 2005, 72, .	3.2	209
10	Intrinsic Rattler-Induced Low Thermal Conductivity in Zintl Type TlInTe₂. Journal of the American Chemical Society, 2017, 139, 4350-4353.	13.7	177
11	Realization of High Thermoelectric FigureÂof Merit in GeTe by Complementary Co-doping of Bi and In. Joule, 2019, 3, 2565-2580.	24.0	175
12	Origin of Enhanced Reducibility/Oxygen Storage Capacity of Ce1-xTixO2Compared to CeO2or TiO2. Chemistry of Materials, 2006, 18, 3249-3256.	6.7	173
13	Engineering ferroelectric instability to achieve ultralow thermal conductivity and high thermoelectric performance in Sn_{1â^'x}Ge_xTe. Energy and Environmental Science, 2019, 12, 589-595.	30.8	155
14	The Origin of Ultralow Thermal Conductivity in InTe: Loneâ€Pairâ€Induced Anharmonic Rattling. Angewandte Chemie - International Edition, 2016, 55, 7792-7796.	13.8	145
15	Borocarbonitrides, BxCyNz. Journal of Materials Chemistry A, 2013, 1, 5806.	10.3	143
16	Localized Vibrations of Bi Bilayer Leading to Ultralow Lattice Thermal Conductivity and High Thermoelectric Performance in Weak Topological Insulator n-Type BiSe. Journal of the American Chemical Society, 2018, 140, 5866-5872.	13.7	137
17	Low Thermal Conductivity and High Thermoelectric Performance in Sb and Bi Codoped GeTe: Complementary Effect of Band Convergence and Nanostructuring. Chemistry of Materials, 2017, 29, 10426-10435.	6.7	117
18	Hydrogen Spillover on CeO₂/Pt: Enhanced Storage of Active Hydrogen. Chemistry of Materials, 2007, 19, 6430-6436.	6.7	97

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19	Localized basis for effective lattice Hamiltonians: Lattice Wannier functions. Physical Review B, 1995, 52, 13236-13246.	3.2	93
20	Intrinsically Ultralow Thermal Conductivity in Ruddlesdenâ€“Popper 2D Perovskite Cs₂PbI₂Cl₂: Localized Anharmonic Vibrations and Dynamic Octahedral Distortions. Journal of the American Chemical Society, 2020, 142, 15595-15603.	13.7	82
21	Bonding heterogeneity and lone pair induced anharmonicity resulted in ultralow thermal conductivity and promising thermoelectric properties in n-type AgPbBiSe₃. Chemical Science, 2019, 10, 4905-4913.	7.4	74
22	Soft Phonon Modes Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance in AgCuTe. Angewandte Chemie - International Edition, 2018, 57, 4043-4047.	13.8	70
23	Thermoelectric properties of materials with nontrivial electronic topology. Journal of Materials Chemistry C, 2015, 3, 12130-12139.	5.5	69
24	Realization of Both n- and p-Type GeTe Thermoelectrics: Electronic Structure Modulation by AgBiSe₂ Alloying. Journal of the American Chemical Society, 2019, 141, 19505-19512.	13.7	69
25	Ferroelectric Instability Induced Ultralow Thermal Conductivity and High Thermoelectric Performance in Rhombohedral p-Type GeSe Crystal. Journal of the American Chemical Society, 2020, 142, 12237-12244.	13.7	69
26	Structural, Optical, and Electronic Properties of Wide Bandgap Perovskites: Experimental and Theoretical Investigations. Journal of Physical Chemistry A, 2016, 120, 3917-3923.	2.5	66
27	Stabilizing nâ€Type Cubic GeSe by Entropyâ€Driven Alloying of AgBiSe₂: Ultralow Thermal Conductivity and Promising Thermoelectric Performance. Angewandte Chemie - International Edition, 2018, 57, 15167-15171.	13.8	66
28	Microscopic Origin of Piezoelectricity in Lead-Free Halide Perovskite: Application in Nanogenerator Design. ACS Energy Letters, 2019, 4, 1004-1011.	17.4	65
29	Machine Learning and Statistical Analysis for Materials Science: Stability and Transferability of Fingerprint Descriptors and Chemical Insights. Chemistry of Materials, 2017, 29, 4190-4201.	6.7	64
30	Ordered Pd₂Ge Intermetallic Nanoparticles as Highly Efficient and Robust Catalyst for Ethanol Oxidation. Chemistry of Materials, 2015, 27, 7459-7467.	6.7	61
31	Ultralow Thermal Conductivity in Chain-like TlSe Due to Inherent Tl⁺ Rattling. Journal of the American Chemical Society, 2019, 141, 20293-20299.	13.7	61
32	Metavalent Bonding in GeSe Leads to High Thermoelectric Performance. Angewandte Chemie - International Edition, 2021, 60, 10350-10358.	13.8	58
33	Photochemical Water Splitting by Bismuth Chalcogenide Topological Insulators. ChemPhysChem, 2017, 18, 2322-2327.	2.1	54
34	Berry curvature dipole senses topological transition in a moirÃ© superlattice. Nature Physics, 2022, 18, 765-770.	16.7	51
35	Intrinsically Low Thermal Conductivity and High Carrier Mobility in Dual Topological Quantum Material, nâ€Type BiTe. Angewandte Chemie - International Edition, 2020, 59, 4822-4829.	13.8	45
36	Operando Generated Ordered Heterogeneous Catalyst for the Selective Conversion of CO₂ to Methanol. ACS Energy Letters, 2021, 6, 509-516.	17.4	41

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37	Mechanistic insights into the promotional effect of Ni substitution in non-noble metal carbides for highly enhanced water splitting. Applied Catalysis B: Environmental, 2021, 298, 120560.	20.2	41
38	Lattice instabilities, anharmonicity and phase transitions in PbZrO3from first principles. Ferroelectrics, 1997, 194, 135-147.	0.6	39
39	Emergence of a weak topological insulator from the BixSey family. Applied Physics Letters, 2017, 110, .	3.3	38
40	Emphanisis in Cubic (SnSe)_{0.5}(AgSbSe₂)_{0.5}: Dynamical Off-Centering of Anion Leads to Low Thermal Conductivity and High Thermoelectric Performance. Journal of the American Chemical Society, 2021, 143, 16839-16848.	13.7	37
41	Ferroelectric phase transitions: A first-principles approach. Ferroelectrics, 1995, 164, 15-32.	0.6	35
42	Engineering the electronic bandgaps and band edge positions in carbon-substituted 2D boron nitride: a first-principles investigation. Physical Chemistry Chemical Physics, 2015, 17, 13547-13552.	2.8	35
43	Intrinsic buckling strength of graphene: First-principles density functional theory calculations. Physical Review B, 2010, 82, .	3.2	30
44	InMnO3: A biferroic. Journal of Applied Physics, 2006, 100, 076104.	2.5	28
45	Local ferroelectricity in thermoelectric SnTe above room temperature driven by competing phonon instabilities and soft resonant bonding. Journal of Materiomics, 2016, 2, 196-202.	5.7	26
46	Transient Species Mediating Energy Transfer to Spin-Forbidden Mn d States in IIâ€“VI Semiconductor Quantum Dots. ACS Energy Letters, 2019, 4, 729-735.	17.4	26
47	First-principles model hamiltonians for ferroelectric phase transitions. Ferroelectrics, 1992, 136, 147-156.	0.6	24
48	Stress-Induced Electronic Structure Modulation of Manganese-Incorporated Ni₂P Leading to Enhanced Activity for Water Splitting. ACS Applied Energy Materials, 2020, 3, 1271-1278.	5.1	24
49	Machine Learning Constrained with Dimensional Analysis and Scaling Laws: Simple, Transferable, and Interpretable Models of Materials from Small Datasets. Chemistry of Materials, 2019, 31, 314-321.	6.7	23
50	Synergetic Effect of Ni-Substituted Pd₂Ge Ordered Intermetallic Nanocomposites for Efficient Electrooxidation of Ethanol in Alkaline Media. ACS Applied Energy Materials, 2019, 2, 7132-7141.	5.1	22
51	Soft Phonon Modes Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance in AgCuTe. Angewandte Chemie, 2018, 130, 4107-4111.	2.0	21
52	Stabilizing nâ€Type Cubic GeSe by Entropyâ€Driven Alloying of AgBiSe₂: Ultralow Thermal Conductivity and Promising Thermoelectric Performance. Angewandte Chemie, 2018, 130, 15387-15391.	2.0	21
53	Unique Features of the Photocatalytic Reduction of H₂O and CO₂ by New Catalysts Based on the Analogues of CdS, Cd₄P₂X₃ (X = Cl, Br, I). ACS Applied Materials & Interfaces, 2018, 10, 2526-2536.	8.0	20
54	Modulation of the electronic structure and thermoelectric properties of orthorhombic and cubic SnSe by AgBiSe₂ alloying. Chemical Science, 2021, 12, 13074-13082.	7.4	20

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55	Intrinsically Low Thermal Conductivity and High Carrier Mobility in Dual Topological Quantum Material, nâ€Type BiTe. Angewandte Chemie, 2020, 132, 4852-4859.	2.0	19
56	Local Symmetry Breaking Suppresses Thermal Conductivity in Crystalline Solids. Angewandte Chemie - International Edition, 2022, 61, .	13.8	16
57	Structure and Properties of Cd₄P₂Cl₃, an Analogue of CdS. Journal of Physical Chemistry C, 2016, 120, 15063-15069.	3.1	13
58	Predicting the DNA Conductance Using a Deep Feedforward Neural Network Model. Journal of Chemical Information and Modeling, 2021, 61, 106-114.	5.4	13
59	Metavalent Bonding in GeSe Leads to High Thermoelectric Performance. Angewandte Chemie, 2021, 133, 10438-10446.	2.0	12
60	Strain coupling in perovskite structural transitions: A first principles approach. Ferroelectrics, 1997, 194, 119-134.	0.6	11
61	First-Principles Theory, Coarse-Grained Models, and Simulations of Ferroelectrics. Accounts of Chemical Research, 2014, 47, 3242-3249.	15.6	10
62	First-principles phonon-based model and theory of martensitic phase transformation in NiTi shape memory alloy. Materialia, 2020, 9, 100602.	2.7	10
63	First-principles model hamiltonians for ferroelectric phase transitions. Ferroelectrics, 1994, 151, 59-68.	0.6	9
64	Enhanced dielectric response of ZrO2 upon Ti doping and introduction of O vacancies. Journal of Applied Physics, 2008, 103, .	2.5	9
65	Destabilizing excitonic insulator phase by pressure tuning of exciton-phonon coupling. Physical Review Research, 2020, 2, .	3.6	9
66	Is There a Lower Size Limit for Superconductivity?. Nano Letters, 2017, 17, 7027-7032.	9.1	8
67	Experimental and first-principles studies of BiVO4/BiV1-xMnxO4-y n-n+ homojunction for efficient charge carrier separation in sunlight induced water splitting. International Journal of Hydrogen Energy, 2018, 43, 15815-15822.	7.1	8
68	Structural Features and HER activity of Cadmium Phosphohalides. Angewandte Chemie - International Edition, 2019, 58, 6926-6931.	13.8	8
69	TiNF and Related Analogues of TiO₂: A Combined Experimental and Theoretical Study. ChemPhysChem, 2018, 19, 3410-3417.	2.1	7
70	Magneto-Optical Stark Effect in Fe-Doped CdS Nanocrystals. Nano Letters, 2021, 21, 3798-3804.	9.1	6
71	Van der Waals hetero-structures of 1H-MoS₂ and N-substituted graphene for catalysis of hydrogen evolution reaction. Materials Research Express, 2019, 6, 124006.	1.6	4
72	Chemical Route to Twisted Graphene, Graphene Oxide and Boron Nitride. Chemistry - A European Journal, 2020, 26, 6499-6503.	3.3	4

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73	Effect of Mn²⁺ substitution on the structure, properties and HER activity of cadmium phosphochlorides. RSC Advances, 2020, 10, 5134-5145.	3.6	4
74	Flat Phonon Band-Based Mechanism of Amorphization of MOF-5 at Ultra-low Pressures. Journal of Physical Chemistry C, 2021, 125, 14924-14931.	3.1	4
75	YRuO3 : A quantum weak ferromagnet. Physical Review Materials, 2020, 4, .	2.4	4
76	Activation of CO₂ and CH₄ on MgO surfaces: mechanistic insights from first-principles theory. Physical Chemistry Chemical Physics, 2022, 24, 1415-1423.	2.8	4
77	Local Symmetry Breaking Suppresses Thermal Conductivity in Crystalline Solids. Angewandte Chemie, 2022, 134, .	2.0	4
78	Unusual CO₂ Adsorption in ZIF-7: Insight from Raman Spectroscopy and Computational Studies. Inorganic Chemistry, 2022, 61, 11571-11580.	4.0	4
79	Origin of the monolayer Raman signature in hexagonal boron nitride: a first-principles analysis. Journal of Physics Condensed Matter, 2018, 30, 185701.	1.8	3
80	CO2 Utilization Through its Reduction to Methanol: Design of Catalysts Using Quantum Mechanics and Machine Learning. , 2022, 7, 1-11.		3
81	Electronic structure and properties of Cd 4 As 2 Br 3 and Cd 4 Sb 2 I 3 , analogues of CdSe and CdTe. Solid State Communications, 2017, 255-256, 5-10.	1.9	2
82	Structural Features and HER activity of Cadmium Phosphohalides. Angewandte Chemie, 2019, 131, 7000-7005.	2.0	2
83	Opportunities and challenges for 2D heterostructures in battery applications: a computational perspective. Nanotechnology, 2022, , .	2.6	1
84	Lattice Instabilities, Anharmonicity and Phase Transitions in PbTiO3 and PbZrO3. Materials Research Society Symposia Proceedings, 1995, 408, 305.	0.1	0
85	Theory and Simulations of Lattice Thermal Conduction. , 2019, , 43-67.		0