

# Umesh V Waghmare

## List of Publications by Year in descending order

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85  
papers

6,462  
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87843

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64755

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87  
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87  
docs citations

87  
times ranked

7962  
citing authors

#	ARTICLE	IF	CITATIONS
1	CO <sub>2</sub> Utilization Through its Reduction to Methanol: Design of Catalysts Using Quantum Mechanics and Machine Learning. , 2022, 7, 1-11.		3
2	Activation of CO <sub>2</sub> and CH <sub>4</sub> on MgO surfaces: mechanistic insights from first-principles theory. Physical Chemistry Chemical Physics, 2022, 24, 1415-1423.	1.3	4
3	Local Symmetry Breaking Suppresses Thermal Conductivity in Crystalline Solids. Angewandte Chemie, 2022, 134, .	1.6	4
4	Local Symmetry Breaking Suppresses Thermal Conductivity in Crystalline Solids. Angewandte Chemie - International Edition, 2022, 61, .	7.2	16
5	Opportunities and challenges for 2D heterostructures in battery applications: a computational perspective. Nanotechnology, 2022, , .	1.3	1
6	Berry curvature dipole senses topological transition in a moiré superlattice. Nature Physics, 2022, 18, 765-770.	6.5	51
7	Unusual CO <sub>2</sub> Adsorption in ZIF-7: Insight from Raman Spectroscopy and Computational Studies. Inorganic Chemistry, 2022, 61, 11571-11580.	1.9	4
8	Predicting the DNA Conductance Using a Deep Feedforward Neural Network Model. Journal of Chemical Information and Modeling, 2021, 61, 106-114.	2.5	13
9	Modulation of the electronic structure and thermoelectric properties of orthorhombic and cubic SnSe by AgBiSe <sub>2</sub> alloying. Chemical Science, 2021, 12, 13074-13082.	3.7	20
10	<i>Operando</i> Generated Ordered Heterogeneous Catalyst for the Selective Conversion of CO <sub>2</sub> to Methanol. ACS Energy Letters, 2021, 6, 509-516.	8.8	41
11	Enhanced atomic ordering leads to high thermoelectric performance in AgSbTe <sub>2</sub> . Science, 2021, 371, 722-727.	6.0	306
12	Metavalent Bonding in GeSe Leads to High Thermoelectric Performance. Angewandte Chemie - International Edition, 2021, 60, 10350-10358.	7.2	58
13	Metavalent Bonding in GeSe Leads to High Thermoelectric Performance. Angewandte Chemie, 2021, 133, 10438-10446.	1.6	12
14	Magneto-Optical Stark Effect in Fe-Doped CdS Nanocrystals. Nano Letters, 2021, 21, 3798-3804.	4.5	6
15	Flat Phonon Band-Based Mechanism of Amorphization of MOF-5 at Ultra-low Pressures. Journal of Physical Chemistry C, 2021, 125, 14924-14931.	1.5	4
16	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.	10.8	41
17	Emphasis in Cubic (SnSe) <sub>0.5</sub> (AgSbSe <sub>2</sub> ) <sub>0.5</sub> : Dynamical Off-Centering of Anion Leads to Low Thermal Conductivity and High Thermoelectric Performance. Journal of the American Chemical Society, 2021, 143, 16839-16848.	6.6	37
18	Intrinsically Ultralow Thermal Conductivity in Ruddlesden-Popper 2D Perovskite Cs <sub>2</sub> PbCl <sub>2</sub> : Localized Anharmonic Vibrations and Dynamic Octahedral Distortions. Journal of the American Chemical Society, 2020, 142, 15595-15603.	6.6	82

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19	Ferroelectric Instability Induced Ultralow Thermal Conductivity and High Thermoelectric Performance in Rhombohedral <i>p</i> -Type GeSe Crystal. <i>Journal of the American Chemical Society</i> , 2020, 142, 12237-12244.	6.6	69
20	Chemical Route to Twisted Graphene, Graphene Oxide and Boron Nitride. <i>Chemistry - A European Journal</i> , 2020, 26, 6499-6503.	1.7	4
21	Scale-free ferroelectricity induced by flat phonon bands in HfO <sub>2</sub> . <i>Science</i> , 2020, 369, 1343-1347.	6.0	231
22	First-principles phonon-based model and theory of martensitic phase transformation in NiTi shape memory alloy. <i>Materialia</i> , 2020, 9, 100602.	1.3	10
23	Intrinsically Low Thermal Conductivity and High Carrier Mobility in Dual Topological Quantum Material, <i>n</i> -Type BiTe. <i>Angewandte Chemie</i> , 2020, 132, 4852-4859.	1.6	19
24	Intrinsically Low Thermal Conductivity and High Carrier Mobility in Dual Topological Quantum Material, <i>n</i> -Type BiTe. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4822-4829.	7.2	45
25	Effect of Mn <sup>2+</sup> substitution on the structure, properties and HER activity of cadmium phosphochlorides. <i>RSC Advances</i> , 2020, 10, 5134-5145.	1.7	4
26	Stress-Induced Electronic Structure Modulation of Manganese-Incorporated Ni <sub>2</sub> P Leading to Enhanced Activity for Water Splitting. <i>ACS Applied Energy Materials</i> , 2020, 3, 1271-1278.	2.5	24
27	Destabilizing excitonic insulator phase by pressure tuning of exciton-phonon coupling. <i>Physical Review Research</i> , 2020, 2, .	1.3	9
28	YRuO <sub>3</sub> : A quantum weak ferromagnet. <i>Physical Review Materials</i> , 2020, 4, .	0.9	4
29	Theory and Simulations of Lattice Thermal Conduction. , 2019, , 43-67.		0
30	Realization of High Thermoelectric Figure of Merit in GeTe by Complementary Co-doping of Bi and In. <i>Joule</i> , 2019, 3, 2565-2580.	11.7	175
31	Synergetic Effect of Ni-Substituted Pd <sub>2</sub> Ge Ordered Intermetallic Nanocomposites for Efficient Electrooxidation of Ethanol in Alkaline Media. <i>ACS Applied Energy Materials</i> , 2019, 2, 7132-7141.	2.5	22
32	Engineering ferroelectric instability to achieve ultralow thermal conductivity and high thermoelectric performance in Sn <sub>1-x</sub> Ge <sub>x</sub> Te. <i>Energy and Environmental Science</i> , 2019, 12, 589-595.	15.6	155
33	Structural Features and HER activity of Cadmium Phosphohalides. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 6926-6931.	7.2	8
34	Microscopic Origin of Piezoelectricity in Lead-Free Halide Perovskite: Application in Nanogenerator Design. <i>ACS Energy Letters</i> , 2019, 4, 1004-1011.	8.8	65
35	Bonding heterogeneity and lone pair induced anharmonicity resulted in ultralow thermal conductivity and promising thermoelectric properties in n-type AgPbBiSe <sub>3</sub> . <i>Chemical Science</i> , 2019, 10, 4905-4913.	3.7	74
36	Structural Features and HER activity of Cadmium Phosphohalides. <i>Angewandte Chemie</i> , 2019, 131, 7000-7005.	1.6	2

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37	Transient Species Mediating Energy Transfer to Spin-Forbidden Mn d States in II-VI Semiconductor Quantum Dots. ACS Energy Letters, 2019, 4, 729-735.	8.8	26
38	Van der Waals hetero-structures of 1H-MoS <sub>2</sub> and N-substituted graphene for catalysis of hydrogen evolution reaction. Materials Research Express, 2019, 6, 124006.	0.8	4
39	Realization of Both n- and p-Type GeTe Thermoelectrics: Electronic Structure Modulation by AgBiSe <sub>2</sub> Alloying. Journal of the American Chemical Society, 2019, 141, 19505-19512.	6.6	69
40	Ultralow Thermal Conductivity in Chain-like TlSe Due to Inherent Tl <sup>+</sup> Rattling. Journal of the American Chemical Society, 2019, 141, 20293-20299.	6.6	61
41	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.	3.2	23
42	Soft Phonon Modes Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance in AgCuTe. Angewandte Chemie - International Edition, 2018, 57, 4043-4047.	7.2	70
43	Soft Phonon Modes Leading to Ultralow Thermal Conductivity and High Thermoelectric Performance in AgCuTe. Angewandte Chemie, 2018, 130, 4107-4111.	1.6	21
44	Origin of the monolayer Raman signature in hexagonal boron nitride: a first-principles analysis. Journal of Physics Condensed Matter, 2018, 30, 185701.	0.7	3
45	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.	6.6	137
46	Unique Features of the Photocatalytic Reduction of H <sub>2</sub> O and CO <sub>2</sub> by New Catalysts Based on the Analogues of CdS, Cd <sub>4</sub> P <sub>2</sub> X <sub>3</sub> (X = Cl, Br, I). ACS Applied Materials & Interfaces, 2018, 10, 2526-2536.	4.0	20
47	TiNF and Related Analogues of TiO <sub>2</sub> : A Combined Experimental and Theoretical Study. ChemPhysChem, 2018, 19, 3410-3417.	1.0	7
48	Stabilizing n-Type Cubic GeSe by Entropy-Driven Alloying of AgBiSe <sub>2</sub> : Ultralow Thermal Conductivity and Promising Thermoelectric Performance. Angewandte Chemie - International Edition, 2018, 57, 15167-15171.	7.2	66
49	Stabilizing n-Type Cubic GeSe by Entropy-Driven Alloying of AgBiSe <sub>2</sub> : Ultralow Thermal Conductivity and Promising Thermoelectric Performance. Angewandte Chemie, 2018, 130, 15387-15391.	1.6	21
50	Experimental and first-principles studies of BiVO <sub>4</sub> /BiV <sub>1-x</sub> MnxO <sub>4-y</sub> n-n+ homojunction for efficient charge carrier separation in sunlight induced water splitting. International Journal of Hydrogen Energy, 2018, 43, 15815-15822.	3.8	8
51	Electronic structure and properties of Cd <sub>4</sub> As <sub>2</sub> Br <sub>3</sub> and Cd <sub>4</sub> Sb <sub>2</sub> I <sub>3</sub> , analogues of CdSe and CdTe. Solid State Communications, 2017, 255-256, 5-10.	0.9	2
52	Intrinsic Rattler-Induced Low Thermal Conductivity in Zintl Type TlInTe <sub>2</sub> . Journal of the American Chemical Society, 2017, 139, 4350-4353.	6.6	177
53	Machine Learning and Statistical Analysis for Materials Science: Stability and Transferability of Fingerprint Descriptors and Chemical Insights. Chemistry of Materials, 2017, 29, 4190-4201.	3.2	64
54	Emergence of a weak topological insulator from the Bi <sub>1-x</sub> Se <sub>y</sub> family. Applied Physics Letters, 2017, 110, .	1.5	38

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55	Is There a Lower Size Limit for Superconductivity?. Nano Letters, 2017, 17, 7027-7032.	4.5	8
56	Photochemical Water Splitting by Bismuth Chalcogenide Topological Insulators. ChemPhysChem, 2017, 18, 2322-2327.	1.0	54
57	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.	3.2	117
58	The Origin of Ultralow Thermal Conductivity in InTe: Lone-Pair-Induced Anharmonic Rattling. Angewandte Chemie - International Edition, 2016, 55, 7792-7796.	7.2	145
59	Structural, Optical, and Electronic Properties of Wide Bandgap Perovskites: Experimental and Theoretical Investigations. Journal of Physical Chemistry A, 2016, 120, 3917-3923.	1.1	66
60	Local ferroelectricity in thermoelectric SnTe above room temperature driven by competing phonon instabilities and soft resonant bonding. Journal of Materiomics, 2016, 2, 196-202.	2.8	26
61	High Power Factor and Enhanced Thermoelectric Performance of SnTe-AgInTe <sub>2</sub> : Synergistic Effect of Resonance Level and Valence Band Convergence. Journal of the American Chemical Society, 2016, 138, 13068-13075.	6.6	214
62	Accurate first-principles structures and energies of diversely bonded systems from an efficient density functional. Nature Chemistry, 2016, 8, 831-836.	6.6	698
63	Structure and Properties of Cd <sub>4</sub> P <sub>2</sub> Cl <sub>3</sub> , an Analogue of CdS. Journal of Physical Chemistry C, 2016, 120, 15063-15069.	1.5	13
64	Thermoelectric properties of materials with nontrivial electronic topology. Journal of Materials Chemistry C, 2015, 3, 12130-12139.	2.7	69
65	Mg Alloying in SnTe Facilitates Valence Band Convergence and Optimizes Thermoelectric Properties. Chemistry of Materials, 2015, 27, 581-587.	3.2	390
66	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.	1.3	35
67	Ordered Pd <sub>2</sub> Ge Intermetallic Nanoparticles as Highly Efficient and Robust Catalyst for Ethanol Oxidation. Chemistry of Materials, 2015, 27, 7459-7467.	3.2	61
68	First-Principles Theory, Coarse-Grained Models, and Simulations of Ferroelectrics. Accounts of Chemical Research, 2014, 47, 3242-3249.	7.6	10
69	Borocarbonitrides, B <sub>x</sub> C <sub>y</sub> N <sub>z</sub> . Journal of Materials Chemistry A, 2013, 1, 5806.	5.2	143
70	Intrinsic buckling strength of graphene: First-principles density functional theory calculations. Physical Review B, 2010, 82, .	1.1	30
71	Synthesis, Structure, and Properties of Boron- and Nitrogen-Doped Graphene. Advanced Materials, 2009, 21, 4726-4730.	11.1	569
72	Enhanced dielectric response of ZrO <sub>2</sub> upon Ti doping and introduction of O vacancies. Journal of Applied Physics, 2008, 103, .	1.1	9

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73	Hydrogen Spillover on $\text{CeO}_2/\text{Pt}$ : Enhanced Storage of Active Hydrogen. Chemistry of Materials, 2007, 19, 6430-6436.	3.2	97
74	Origin of Enhanced Reducibility/Oxygen Storage Capacity of $\text{Ce}_{1-x}\text{Ti}_x\text{O}_2$ Compared to $\text{CeO}_2$ or $\text{TiO}_2$ . Chemistry of Materials, 2006, 18, 3249-3256.	3.2	173
75	$\text{InMnO}_3$ : A biferroic. Journal of Applied Physics, 2006, 100, 076104.	1.1	28
76	Biferroic $\text{YCrO}_3$ . Physical Review B, 2005, 72, .	1.1	209
77	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, .	1.1	299
78	Ab initio statistical mechanics of the ferroelectric phase transition in $\text{PbTiO}_3$ . Physical Review B, 1997, 55, 6161-6173.	1.1	308
79	Lattice instabilities, anharmonicity and phase transitions in $\text{PbZrO}_3$ from first principles. Ferroelectrics, 1997, 194, 135-147.	0.3	39
80	Strain coupling in perovskite structural transitions: A first principles approach. Ferroelectrics, 1997, 194, 119-134.	0.3	11
81	Lattice Instabilities, Anharmonicity and Phase Transitions in $\text{PbTiO}_3$ and $\text{PbZrO}_3$ . Materials Research Society Symposia Proceedings, 1995, 408, 305.	0.1	0
82	Localized basis for effective lattice Hamiltonians: Lattice Wannier functions. Physical Review B, 1995, 52, 13236-13246.	1.1	93
83	Ferroelectric phase transitions: A first-principles approach. Ferroelectrics, 1995, 164, 15-32.	0.3	35
84	First-principles model hamiltonians for ferroelectric phase transitions. Ferroelectrics, 1994, 151, 59-68.	0.3	9
85	First-principles model hamiltonians for ferroelectric phase transitions. Ferroelectrics, 1992, 136, 147-156.	0.3	24