

Manish Agarwal

List of Publications by Year in descending order

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39
papers

1,101
citations

331670

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395702

33
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docs citations

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times ranked

1128
citing authors

#	ARTICLE	IF	CITATIONS
1	Role of Reduced CeO ₂ (110) Surface for CO ₂ Reduction to CO and Methanol. Journal of Physical Chemistry C, 2016, 120, 16626-16635.	3.1	93
2	Relationship between Structure, Entropy, and Diffusivity in Water and Water-Like Liquids. Journal of Physical Chemistry B, 2010, 114, 6995-7001.	2.6	84
3	Thermodynamic, Diffusional, and Structural Anomalies in Rigid-Body Water Models. Journal of Physical Chemistry B, 2011, 115, 6935-6945.	2.6	79
4	Estimating the entropy of liquids from atom-atom radial distribution functions: silica, beryllium fluoride and water. Molecular Physics, 2008, 106, 1925-1938.	1.7	57
5	Tetrahedral order, pair correlation entropy, and waterlike liquid state anomalies: Comparison of GeO ₂ with BeF ₂ , SiO ₂ , and H ₂ O. Journal of Chemical Physics, 2010, 132, 234507.	3.0	55
6	Local Order, Energy, and Mobility of Water Molecules in the Hydration Shell of Small Peptides. Journal of Physical Chemistry B, 2010, 114, 651-659.	2.6	52
7	Comparison of Tetrahedral Order, Liquid State Anomalies, and Hydration Behavior of mTIP3P and TIP4P Water Models. Journal of Chemical Theory and Computation, 2011, 7, 3354-3367.	5.3	52
8	Relationship between structure, entropy, and mobility in network-forming ionic melts. Physical Review E, 2009, 79, 030202.	2.1	49
9	Ionic melts with waterlike anomalies: Thermodynamic properties of liquid BeF ₂ . Journal of Chemical Physics, 2007, 127, 164502.	3.0	46
10	Waterlike Structural and Excess Entropy Anomalies in Liquid Beryllium Fluoride. Journal of Physical Chemistry B, 2007, 111, 13294-13300.	2.6	44
11	Enhanced Polymeric Dielectrics through Incorporation of Hydroxyl Groups. Macromolecules, 2014, 47, 1122-1129.	4.8	43
12	Excess entropy scaling of transport properties in network-forming ionic melts (SiO ₂ and BeF ₂). Journal of Chemical Physics, 2011, 134, 014502.	3.0	40
13	Transport Properties of Tetrahedral, Network-Forming Ionic Melts. Journal of Physical Chemistry B, 2009, 113, 15284-15292.	2.6	37
14	Reformulation of Gasoline To Replace Aromatics by Biomass-Derived Alkyl Levulinates. ACS Sustainable Chemistry and Engineering, 2017, 5, 7118-7127.	6.7	33
15	Artificial intelligence and machine learning in glass science and technology: 21 challenges for the 21 st century. International Journal of Applied Glass Science, 2021, 12, 277-292.	2.0	28
16	Paradoxical Effect of Trehalose on the Aggregation of I ⁺ -Synuclein: Expedites Onset of Aggregation yet Reduces Fibril Load. ACS Chemical Neuroscience, 2018, 9, 1477-1491.	3.5	27
17	Oxygen anion diffusion in double perovskite GdBaCo ₂ O ₅ + δ and LnBa _{0.5} Sr _{0.5} Co ₂ xFe _x O ₅ + δ (Ln=Agd, Pr). Tj ETQq1 1 0.784314 rsgB	7.1	26
18	Looking through glass: Knowledge discovery from materials science literature using natural language processing. Patterns, 2021, 2, 100290.	5.9	25

#	ARTICLE	IF	CITATIONS
19	Controlling surface cation segregation in a nanostructured double perovskite $\text{GdBaCo}_{2-x}\text{O}_{5+\delta}$ electrode for solid oxide fuel cells. <i>Nanoscale</i> , 2019, 11, 21404-21418.	5.6	24
20	Structural correlations and cooperative dynamics in supercooled liquids. <i>Journal of Chemical Physics</i> , 2012, 137, 024508.	3.0	23
21	Identifying the Origin of the Limiting Process in a Double Perovskite $\text{PrBa}_{0.5}\text{Sr}_{0.5}\text{Co}_{1.5}\text{Fe}_{0.5}\text{O}_{5+\delta}$ Thin-Film Electrode for Solid Oxide Fuel Cells. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 25243-25253.	8.0	23
22	Redox Sensitive Self-Assembling Dipeptide for Sustained Intracellular Drug Delivery. <i>Bioconjugate Chemistry</i> , 2019, 30, 2458-2468.	3.6	19
23	Evidence of a two-dimensional glass transition in graphene: Insights from molecular simulations. <i>Scientific Reports</i> , 2019, 9, 4517.	3.3	19
24	Structure and transport properties of $\text{LiF} \cdot \text{BeF}_2$ mixtures: Comparison of rigid and polarizable ion potentials#. <i>Journal of Chemical Sciences</i> , 2012, 124, 261-269.	1.5	15
25	Effective interactions between nanoparticles: Creating temperature-independent solvation environments for self-assembly. <i>Journal of Chemical Physics</i> , 2016, 144, 244901.	3.0	13
26	Non-bonding and bonding interactions of biogenic impurities with the metal catalyst and the design of bimetallic alloys. <i>Journal of Catalysis</i> , 2017, 352, 542-556.	6.2	13
27	Dielectric permittivity enhancement in hydroxyl functionalized polyolefins via cooperative interactions with water. <i>Applied Physics Letters</i> , 2013, 102, 152901.	3.3	11
28	A Carâ€Parrinello Molecular Dynamics Simulation Study of the Retro Dielsâ€Alder Reaction for Partially Saturated 2-Pyrones in Water. <i>Journal of Physical Chemistry C</i> , 2018, 122, 11599-11607.	3.1	11
29	Understanding the Nature of Amino Acid Interactions with Pd(111) or Pdâ€Au Bimetallic Catalysts in the Aqueous Phase. <i>Langmuir</i> , 2018, 34, 1300-1310.	3.5	10
30	GPUâ€accelerated direct numerical simulations of decaying compressible turbulence employing a GKMAâ€based solver. <i>International Journal for Numerical Methods in Fluids</i> , 2017, 83, 737-754.	1.6	9
31	Mechanistic Elucidation of Surface Cation Segregation in Double Perovskite $\text{PrBaCo}_2\text{O}_{5+\delta}$ Material using MD and DFT Simulations for Solid Oxide Fuel Cells. <i>Ionics</i> , 2020, 26, 1307-1314.	2.4	9
32	Elucidating the role of solvents in acid catalyzed dehydration of biorenewable hydroxy-lactones. <i>Reaction Chemistry and Engineering</i> , 2020, 5, 651-662.	3.7	7
33	Thermodynamic regimes over which homologous alkane fluids can be treated as simple liquids. <i>Journal of Molecular Liquids</i> , 2017, 231, 106-115.	4.9	6
34	Effect of Fe-Doping on Oxygen Anion Diffusion in $\text{PrBaCo}_{2-x}\text{Fe}_x\text{O}_{5+\delta}$ Double Perovskite Electrodes for Solid Oxide Fuel Cells. <i>ECS Transactions</i> , 2017, 77, 125-131.	0.5	6
35	Stressâ€Strain Relationships in Hydroxyl Substituted Polyethylene. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7598-7605.	2.6	5
36	Evaluation of collective transport properties of ionic melts from molecular dynamics simulations. <i>Journal of Chemical Sciences</i> , 2009, 121, 913-919.	1.5	4

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37	Nanoparticle Synthesis and Oxygen Anion Diffusion in Double Perovskite $\text{GdBaCo}_{2-x}\text{Fe}_x\text{O}_{5+\delta}$ Electrodes for SOFC. ECS Transactions, 2016, 72, 111-116.	0.5	2
38	Ca-Doped Double Perovskite $\text{PrBa}_{0.8}\text{Ca}_{0.2}\text{Co}_2\text{O}_{5+\delta}$ Thin-Film Electrodes: Experimental and Theoretical Study. ECS Transactions, 2017, 78, 499-506.	0.5	2
39	Noncovalent Interactions of Biogenic Impurities with Transition Metal Catalyst Surfaces. RSC Catalysis Series, 2019, , 527-547.	0.1	0