Manish Agarwal

List of Publications by Year
in descending order

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39 papers	1,101 citations	331670 21 h-index	395702 33 g-index
39 all docs	39 docs citations	39 times ranked	1128 citing authors

#	Article	IF	Citations
1	Artificial intelligence and machine learning in glass science and technology: 21 challenges for the 21st century. International Journal of Applied Glass Science, 2021, 12, 277-292.	2.0	28
2	Looking through glass: Knowledge discovery from materials science literature using natural language processing. Patterns, 2021, 2, 100290.	5.9	25
3	Mechanistic Elucidation of Surface Cation Segregation in Double Perovskite PrBaCo2O5+Î´ Material using MD and DFT Simulations for Solid Oxide Fuel Cells. Ionics, 2020, 26, 1307-1314.	2.4	9
4	Elucidating the role of solvents in acid catalyzed dehydration of biorenewable hydroxy-lactones. Reaction Chemistry and Engineering, 2020, 5, 651-662.	3.7	7
5	Redox Sensitive Self-Assembling Dipeptide for Sustained Intracellular Drug Delivery. Bioconjugate Chemistry, 2019, 30, 2458-2468.	3.6	19
6	Identifying the Origin of the Limiting Process in a Double Perovskite PrBa_{0.5}Sr_{0.5}Co_{1.5}Fe_{0.5}O_{5+Î´} Thin-Film Electrode for Solid Oxide Fuel Cells. ACS Applied Materials & Interfaces, 2019, 11, 25243-25253.	8.0	23
7	Evidence of a two-dimensional glass transition in graphene: Insights from molecular simulations. Scientific Reports, 2019, 9, 4517.	3.3	19
8	Controlling surface cation segregation in a nanostructured double perovskite GdBaCo₂O_{5+Î´} electrode for solid oxide fuel cells. Nanoscale, 2019, 11, 21404-21418.	5.6	24
9	Noncovalent Interactions of Biogenic Impurities with Transition Metal Catalyst Surfaces. RSC Catalysis Series, 2019, , 527-547.	0.1	0
10	Understanding the Nature of Amino Acid Interactions with Pd(111) or Pdâ€“Au Bimetallic Catalysts in the Aqueous Phase. Langmuir, 2018, 34, 1300-1310.	3.5	10
11	Paradoxical Effect of Trehalose on the Aggregation of Î±-Synuclein: Expedites Onset of Aggregation yet Reduces Fibril Load. ACS Chemical Neuroscience, 2018, 9, 1477-1491.	3.5	27
12	A Carâ€“Parrinello Molecular Dynamics Simulation Study of the Retro Dielsâ€“Alder Reaction for Partially Saturated 2-Pyrones in Water. Journal of Physical Chemistry C, 2018, 122, 11599-11607.	3.1	11
13	Thermodynamic regimes over which homologous alkane fluids can be treated as simple liquids. Journal of Molecular Liquids, 2017, 231, 106-115.	4.9	6
14	Effect of Fe-Doping on Oxygen Anion Diffusion in PrBaCo _{2-x} Fe _x O _{5+Î´} Double Perovskite Electrodes for Solid Oxide Fuel Cells. ECS Transactions, 2017, 77, 125-131.	0.5	6
15	Ca-Doped Double Perovskite PrBa_{0.8}Ca_{0.2}Co₂O_{5+Î´}Thin-Film Electrodes: Experimental and Theoretical Study. ECS Transactions, 2017, 78, 499-506.	0.5	2
16	Non-bonding and bonding interactions of biogenic impurities with the metal catalyst and the design of bimetallic alloys. Journal of Catalysis, 2017, 352, 542-556.	6.2	13
17	Reformulation of Gasoline To Replace Aromatics by Biomass-Derived Alkyl Levulinates. ACS Sustainable Chemistry and Engineering, 2017, 5, 7118-7127.	6.7	33
18	GPUâ€accelerated direct numerical simulations of decaying compressible turbulence employing a GKMâ€based solver. International Journal for Numerical Methods in Fluids, 2017, 83, 737-754.	1.6	9

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19	Stressâ€“Strain Relationships in Hydroxyl Substituted Polyethylene. Journal of Physical Chemistry B, 2016, 120, 7598-7605.	2.6	5
20	Effective interactions between nanoparticles: Creating temperature-independent solvation environments for self-assembly. Journal of Chemical Physics, 2016, 144, 244901.	3.0	13
21	Oxygen anion diffusion in double perovskite GdBaCo2O5+Î´ and LnBa0.5Sr0.5Co2âˆ’xFexO5+Î´ (LnÂ=ÂGd, Pr,) Tj ETQq1 1 0.784314 r	7.1	26
22	Role of Reduced CeO₂(110) Surface for CO₂ Reduction to CO and Methanol. Journal of Physical Chemistry C, 2016, 120, 16626-16635.	3.1	93
23	Nanoparticle Synthesis and Oxygen Anion Diffusion in Double Perovskite GdBaCo_{2-x}Fe_xO_{5+Î´} Electrodes for SOFC. ECS Transactions, 2016, 72, 111-116.	0.5	2
24	Enhanced Polymeric Dielectrics through Incorporation of Hydroxyl Groups. Macromolecules, 2014, 47, 1122-1129.	4.8	43
25	Dielectric permittivity enhancement in hydroxyl functionalized polyolefins via cooperative interactions with water. Applied Physics Letters, 2013, 102, 152901.	3.3	11
26	Structural correlations and cooperative dynamics in supercooled liquids. Journal of Chemical Physics, 2012, 137, 024508.	3.0	23
27	Structure and transport properties of LiFâ€“BeF2 mixtures: Comparison of rigid and polarizable ion potentials#. Journal of Chemical Sciences, 2012, 124, 261-269.	1.5	15
28	Thermodynamic, Diffusional, and Structural Anomalies in Rigid-Body Water Models. Journal of Physical Chemistry B, 2011, 115, 6935-6945.	2.6	79
29	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
30	Excess entropy scaling of transport properties in network-forming ionic melts (SiO2 and BeF2). Journal of Chemical Physics, 2011, 134, 014502.	3.0	40
31	Tetrahedral order, pair correlation entropy, and waterlike liquid state anomalies: Comparison of GeO2 with BeF2, SiO2, and H2O. Journal of Chemical Physics, 2010, 132, 234507.	3.0	55
32	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
33	Relationship between Structure, Entropy, and Diffusivity in Water and Water-Like Liquids. Journal of Physical Chemistry B, 2010, 114, 6995-7001.	2.6	84
34	Relationship between structure, entropy, and mobility in network-forming ionic melts. Physical Review E, 2009, 79, 030202.	2.1	49
35	Evaluation of collective transport properties of ionic melts from molecular dynamics simulations. Journal of Chemical Sciences, 2009, 121, 913-919.	1.5	4
36	Transport Properties of Tetrahedral, Network-Forming Ionic Melts. Journal of Physical Chemistry B, 2009, 113, 15284-15292.	2.6	37

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37	Estimating the entropy of liquids from atomâ€“atom radial distribution functions: silica, beryllium fluoride and water. Molecular Physics, 2008, 106, 1925-1938.	1.7	57
38	Ionic melts with waterlike anomalies: Thermodynamic properties of liquid BeF2. Journal of Chemical Physics, 2007, 127, 164502.	3.0	46
39	Waterlike Structural and Excess Entropy Anomalies in Liquid Beryllium Fluoride. Journal of Physical Chemistry B, 2007, 111, 13294-13300.	2.6	44