

Yashonath Subramanian

List of Publications by Year in descending order

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149
papers

2,935
citations

159358

30
h-index

214527

47
g-index

151
all docs

151
docs citations

151
times ranked

1909
citing authors

#	ARTICLE	IF	CITATIONS
1	Ionic conduction in the solid state. <i>Journal of Chemical Sciences</i> , 2006, 118, 135-154.	0.7	157
2	Diffusion of Sorbates in Zeolites Y and A: Novel Dependence on Sorbate Size and Strength of Sorbate-Zeolite Interaction. <i>The Journal of Physical Chemistry</i> , 1994, 98, 6368-6376.	2.9	146
3	Localization and mobility of benzene in sodium-Y zeolite by molecular dynamics calculations. <i>The Journal of Physical Chemistry</i> , 1989, 93, 5016-5019.	2.9	144
4	The siting, energetics and mobility of saturated hydrocarbons inside zeolitic cages: methane in zeolite Y. <i>Nature</i> , 1988, 331, 601-604.	13.7	122
5	A Monte Carlo study of crystal structure transformations. <i>Molecular Physics</i> , 1985, 54, 245-251.	0.8	95
6	A molecular dynamics study of methane in zeolite NaY. <i>Chemical Physics Letters</i> , 1988, 153, 551-556.	1.2	93
7	Estimation of Error in the Diffusion Coefficient from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5437-5445.	1.2	71
8	Diffusion Anomaly in Silicalite and VPI-5 from Molecular Dynamics Simulations. <i>The Journal of Physical Chemistry</i> , 1995, 99, 4286-4292.	2.9	66
9	Diffusion Anomaly as a Function of Molecular Length of Linear Molecules: A Levitation Effect. <i>Journal of the American Chemical Society</i> , 2003, 125, 7116-7123.	6.6	64
10	Molecularly adsorbed oxygen on metals: electron spectroscopic studies. <i>Chemical Physics Letters</i> , 1982, 88, 13-16.	1.2	62
11	A six-site anisotropic atom-atom potential model for the condensed phases of benzene. <i>Molecular Physics</i> , 1988, 64, 361-376.	0.8	61
12	A molecular dynamics study of xenon sorbed in sodium Y zeolite. 1. Temperature and concentration dependence. <i>The Journal of Physical Chemistry</i> , 1992, 96, 10469-10477.	2.9	52
13	Diffusion in zeolites: Anomalous dependence on sorbate diameter. <i>Journal of Chemical Physics</i> , 1994, 100, 4013-4016.	1.2	45
14	Diffusion in Nanoporous Phases: A Size Dependence and Levitation Effect. <i>Journal of Physical Chemistry B</i> , 2008, 112, 665-686.	1.2	45
15	Diffusion of Propane in Zeolite NaY: A Molecular Dynamics and Quasi-Elastic Neutron Scattering Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 527-533.	1.2	44
16	Structure, Conductivity, and Ionic Motion in Na _{1+x} Zr ₂ Si ₆ P ₃ -xO ₁₂ : A Simulation Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7081-7089.	1.2	40
17	Breakdown of the Stokes-Einstein Relationship: Role of Interactions in the Size Dependence of Self-Diffusivity. <i>Journal of Physical Chemistry B</i> , 2006, 110, 17207-17211.	1.2	40
18	Xenon in sodium Y zeolite. 2. Arrhenius relation, mechanism, and barrier height distribution for cage-to-cage diffusion. <i>The Journal of Physical Chemistry</i> , 1993, 97, 3849-3857.	2.9	39

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19	Structure and Dynamics of Benzene in One-Dimensional Channels. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11977-11986.	1.2	38
20	Structural Insights into Proton Conduction in Gallic Acid–Isoniazid Cocrystals. <i>Crystal Growth and Design</i> , 2014, 14, 423-426.	1.4	38
21	Rotation driven translational diffusion of polyatomic ions in water: A novel mechanism for breakdown of Stokes-Einstein relation. <i>Journal of Chemical Physics</i> , 2017, 146, 164502.	1.2	38
22	Size-Dependent Maximum in Ion Conductivity: The Levitation Effect Provides an Alternative Explanation. <i>Journal of Physical Chemistry B</i> , 2005, 109, 8120-8124.	1.2	37
23	A molecular dynamics study of cage-to-cage migration in sodium Y zeolite: role of surface-mediated diffusion. <i>The Journal of Physical Chemistry</i> , 1991, 95, 5877-5881.	2.9	36
24	Diffusion of Pure CH ₄ and Its Binary Mixture with CO ₂ in Faujasite NaY: A Combination of Neutron Scattering Experiments and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2010, 114, 5027-5034.	1.5	35
25	Levitation effect in zeolites: Quasielastic neutron scattering and molecular dynamics study of pentane isomers in zeolite NaY. <i>Journal of Chemical Physics</i> , 2010, 132, 144507.	1.2	34
26	Relation Between the Diffusivity, Viscosity, and Ionic Radius of LiCl in Water, Methanol, and Ethylene Glycol: A Molecular Dynamics Simulation. <i>Journal of Physical Chemistry B</i> , 2013, 117, 8196-8208.	1.2	34
27	Surprising diffusion behaviour in the restricted regions of silicalite. <i>Chemical Physics Letters</i> , 1994, 228, 284-288.	1.2	33
28	Influence of non-geometrical factors on intracrystalline diffusion. <i>Molecular Physics</i> , 1993, 78, 1-6.	0.8	31
29	n-Pentane and Isopentane in One-Dimensional Channels. <i>Journal of the American Chemical Society</i> , 2003, 125, 7425-7434.	6.6	31
30	Dependence of the self-diffusion coefficient on the sorbate concentration: A two-dimensional lattice gas model with and without confinement. <i>Journal of Chemical Physics</i> , 1999, 111, 1658-1667.	1.2	30
31	Levitation effect and its relationship with the underlying potential energy landscape. <i>Journal of Chemical Physics</i> , 1999, 110, 5960-5968.	1.2	29
32	The Stokes–Einstein Relationship and the Levitation Effect: Size-Dependent Diffusion Maximum in Dense Fluids and Close-Packed Disordered Solids. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5824-5835.	1.2	28
33	Transport in nanoporous zeolites: Relationships between sorbate size, entropy, and diffusivity. <i>Journal of Chemical Physics</i> , 2012, 136, 174510.	1.2	27
34	High Interfacial Barriers at Narrow Carbon Nanotube–Water Interfaces. <i>Langmuir</i> , 2018, 34, 8099-8111.	1.6	27
35	Temperature dependence of the levitation effect Implications for separation of multicomponent mixtures. <i>Faraday Discussions</i> , 1997, 106, 105-118.	1.6	26
36	Coupled jump rotational dynamics in aqueous nitrate solutions. <i>Journal of Chemical Physics</i> , 2016, 145, 234502.	1.2	26

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37	Lithium Ion Motion in LiZr ₂ (PO ₄) ₃ . Journal of Physical Chemistry B, 2001, 105, 6785-6791.	1.2	24
38	Orientational preference and influence of rotation on methane mobility in one-dimensional channels. Journal of Chemical Physics, 2002, 116, 2175-2183.	1.2	24
39	A Full Interionic Potential for Na _{1+x} Zr ₂ SixP _{3-x} O ₁₂ Superionic Conductors. Journal of the American Chemical Society, 2002, 124, 3828-3829.	6.6	24
40	Concentration Dependent Self-Assembly of TrK-NGF Receptor Derived Tripeptide: New Insights from Experiment and Computer Simulations. Journal of Physical Chemistry B, 2017, 121, 815-824.	1.2	24
41	Evidence in Support of Levitation Effect as the Reason for Size Dependence of Ionic Conductivity in Water: A Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2006, 110, 12179-12190.	1.2	22
42	Types of Dependence of Self-Diffusivity on Sorbate Concentration in Parameter Space: A Two-Dimensional Lattice Gas Study. Journal of Physical Chemistry B, 2000, 104, 2607-2612.	1.2	21
43	Correlation between conductivity or diffusivity and activation energy in amorphous solids. Journal of Chemical Physics, 2008, 129, 144103.	1.2	20
44	Mutual diffusion in a binary Ar-Kr mixture confined within zeolite NaY. Physical Review E, 2002, 65, 061202.	0.8	19
45	Pressure Induced Orientational Ordering in p-Terphenyl. Journal of Physical Chemistry B, 2005, 109, 1433-1440.	1.2	19
46	Structure and dynamics of polar liquids: A molecular dynamics investigation of N,N-dimethyl formamide. Chemical Physics, 1991, 155, 351-356.	0.9	18
47	Adsorption of xenon in zeolite Y: a molecular dynamics study. Chemical Physics Letters, 1991, 177, 54-58.	1.2	18
48	Study of Translational and Rotational Mobility and Orientational Preference of Ethane in One-Dimensional Channels. Journal of Physical Chemistry A, 2002, 106, 7130-7137.	1.1	18
49	High Pressure Phase of Biphenyl at Room Temperature: A Monte Carlo Study. Journal of Physical Chemistry B, 2004, 108, 4178-4184.	1.2	18
50	Molecular dynamics investigation of sorption of argon in NaCaA zeolite. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1063.	1.7	17
51	Levitation Effect: Distinguishing Anomalous from Linear Regime of Guests Sorbed in Zeolites through the Decay of Intermediate Scattering Function and Wavevector Dependence of Self-Diffusivity. Journal of Physical Chemistry B, 2005, 109, 3979-3983.	1.2	17
52	Monte Carlo simulation of the crystal to plastic crystal transition in carbon tetrachloride. Chemical Physics Letters, 1985, 119, 22-28.	1.2	16
53	Probing Potential Energy Surfaces in Confined Systems: Behavior of Mean-Square Displacement in Zeolites. The Journal of Physical Chemistry, 1994, 98, 9354-9359.	2.9	16
54	Ion Mobility and Levitation Effect: Anomalous Diffusion in Nasicon-Type Structure. Journal of Physical Chemistry B, 2002, 106, 3443-3448.	1.2	16

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55	Charge transfer in Chevrel phases. <i>Solid State Communications</i> , 1981, 37, 325-327.	0.9	15
56	Anomalous behaviour of cage-to-cage diffusion of methane in zeolites A and Y. <i>Chemical Physics Letters</i> , 1994, 223, 363-368.	1.2	15
57	Neutron Scattering and Molecular Dynamics Evidence for Levitation Effect in Nanopores. <i>Journal of Physical Chemistry B</i> , 2009, 113, 12635-12638.	1.2	15
58	Effect of a Distribution of Pore Dimension on Levitation Effect. <i>Journal of Physical Chemistry B</i> , 2000, 104, 9126-9130.	1.2	14
59	Acetylene diffusion in Na-Y zeolite. <i>Pramana - Journal of Physics</i> , 2004, 63, 449-453.	0.9	14
60	Structure, Energetics, and Dynamics of Pedal-Like Motion in Stilbene from Molecular Simulation and ab Initio Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 17403-17411.	1.2	14
61	Diffusion of 1,3-butadiene adsorbed in Na-Y zeolite: Neutron scattering study. <i>Chemical Physics Letters</i> , 2007, 442, 311-315.	1.2	14
62	Hexane Isomers in Faujasite: Anomalous Diffusion and Kinetic Separation. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14745-14756.	1.5	14
63	Using porphyrin-amino acid pairs to model the electrochemistry of heme proteins: experimental and theoretical investigations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10018-10029.	1.3	14
64	Anomalous diffusion of linear and branched pentanes within zeolite NaY. <i>Molecular Physics</i> , 2004, 102, 1057-1066.	0.8	13
65	Distinct Diffusion in Binary Mixtures Confined in Slit Graphite Pores. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4411-4421.	1.2	13
66	Ionic conductivity in aqueous electrolyte solutions: Insights from computer simulations. <i>Journal of Molecular Liquids</i> , 2019, 277, 506-515.	2.3	13
67	Molecular dynamics simulation of clathrates: noble gases in the cages of β -hydroquinone. <i>Chemical Physics Letters</i> , 1992, 192, 390-394.	1.2	12
68	Diffusion behaviour of binary mixtures in restricted regions of zeolite NaY from molecular dynamics calculations. <i>Chemical Physics Letters</i> , 1995, 234, 16-20.	1.2	12
69	Pressure-Induced Ordering in Adamantane: A Monte Carlo Simulation Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 2014-2020.	1.2	12
70	Existence of a Size-Dependent Diffusivity Maximum for Uncharged Solutes in Water and Its Implications. <i>Journal of Physical Chemistry B</i> , 2006, 110, 12072-12079.	1.2	12
71	Conformation of confined alkanes: n-butane in zeolite Y. <i>Journal of Chemical Physics</i> , 1996, 105, 7223-7226.	1.2	11
72	Conformational Analysis of n-Butane in Zeolite NaCaA: Temperature and Concentration Dependence. <i>Journal of Physical Chemistry B</i> , 1997, 101, 5675-5683.	1.2	11

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73	Translational-orientational coupling during passage of methane through the bottleneck in zeolite A. <i>Journal of Chemical Physics</i> , 2001, 114, 11.	1.2	11
74	Estimation of slow diffusion rates in confined systems: CCl ₄ in zeolite NaA. <i>Molecular Physics</i> , 2002, 100, 641-647.	0.8	11
75	Diffusion processes in a poly-crystalline zeolitic material: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2018, 149, 064702.	1.2	11
76	Structure-potential relationship and nature of disorder in liquids and glassy solids. <i>Chemical Physics Letters</i> , 1992, 189, 311-315.	1.2	10
77	Monte Carlo and molecular dynamics simulation of argon clusters and n-alkanes in the confined regions of zeolites. <i>Bulletin of Materials Science</i> , 1997, 20, 845-878.	0.8	10
78	Diffusion anomaly from analytical formula. <i>Journal of Chemical Physics</i> , 2000, 112, 965-969.	1.2	10
79	A molecular dynamics study of ambient and high pressure phases of silica: Structure and enthalpy variation with molar volume. <i>Journal of Chemical Physics</i> , 2014, 140, 244512.	1.2	10
80	Separating Hydrocarbon Mixtures by Driving the Components in Opposite Directions: High Degree of Separation Factor and Energy Efficiency. <i>Physical Review Letters</i> , 2020, 124, 255901.	2.9	10
81	Dynamics of adsorbates in micropores of zeolites and breakdown of Arrhenius behavior. <i>Physical Review B</i> , 1992, 45, 10095-10098.	1.1	9
82	Separation of multi-component mixtures by the use of the anomalous regime in the diffusivity. <i>Molecular Physics</i> , 2000, 98, 657-665.	0.8	9
83	Rotation of propane molecules in supercages of Na-Y zeolite. <i>Chemical Physics</i> , 2003, 292, 217-222.	0.9	9
84	Translational and rotational diffusion of SF ₆ in zeolite NaY. <i>Journal of Chemical Physics</i> , 2004, 120, 5315-5321.	1.2	9
85	Diffusion Anomaly at Low Temperatures in Confined Systems from the Rare Events Method. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7098-7101.	1.2	9
86	Mode coupling theory analysis of electrolyte solutions: Time dependent diffusion, intermediate scattering function, and ion solvation dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 124502.	1.2	9
87	Influence of a Counterion on the Ion Atmosphere of an Anion: A Molecular Dynamics Study of LiX and CsX (X = F ⁻ , Cl ⁻ , I ⁻) in Methanol. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10921-10933.	1.2	9
88	Simulations on "Powder" Samples for Better Agreement with Macroscopic Measurements. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16172-16178.	1.5	9
89	Dependence of diffusion properties in zeolites Y and A: a search in the sorbate interaction parameter space. <i>Molecular Physics</i> , 1997, 90, 889-894.	0.8	8
90	Levitation Effect and Its Dependence on Sorbate Concentration. <i>Journal of Physical Chemistry B</i> , 1997, 101, 8035-8037.	1.2	8

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91	High-Pressure Study of Adamantane: Variable Shape Simulations up to 26 GPa. <i>Journal of Physical Chemistry B</i> , 2005, 109, 17296-17303.	1.2	8
92	Ions in water: Role of attractive interactions in size dependent diffusivity maximum. <i>Journal of Chemical Physics</i> , 2010, 133, 114504.	1.2	8
93	A molecular dynamics study and molecular level explanation of pressure dependence of ionic conductivity of potassium chloride in water. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10877.	1.3	8
94	Effect of interionic interactions on the structure and dynamics of ionic solvation shells in aqueous electrolyte solutions. <i>RSC Advances</i> , 2016, 6, 114666-114675.	1.7	8
95	Bridging the gap between diffusivities from experiment and molecular dynamics: n-hexane and 2,2-dimethyl butane in zeolite BEA. <i>Microporous and Mesoporous Materials</i> , 2019, 287, 124-134.	2.2	8
96	Plastic and glassy crystalline states of methane: A Monte Carlo simulation study. <i>Chemical Physics Letters</i> , 1983, 101, 524-527.	1.2	7
97	A Monte Carlo study of the condensed phases of biphenyl. <i>Molecular Physics</i> , 1995, 84, 49-68.	0.8	7
98	Inverse Surface Melting in Confined Clusters: Ar ₁₃ in Zeolite L. <i>Journal of Physical Chemistry B</i> , 1997, 101, 389-395.	1.2	7
99	Adsorption Isotherm and Other Properties of Methane in Zeolite A from an Intermolecular Potential Derived from ab Initio Calculations. <i>Journal of the American Chemical Society</i> , 2003, 125, 16192-16193.	6.6	7
100	Large Distinct Diffusivity in Binary Mixtures Confined to Zeolite NaY. <i>Journal of Physical Chemistry B</i> , 2005, 109, 22092-22095.	1.2	7
101	A comparative molecular dynamics study of diffusion of n-decane and 3-methyl pentane in Y zeolite. <i>Journal of Chemical Sciences</i> , 2009, 121, 921-927.	0.7	7
102	Dependence of diffusivity on density and solute diameter in liquid phase: A molecular dynamics study of Lennard-Jones system. <i>Journal of Chemical Physics</i> , 2012, 136, 144505.	1.2	7
103	Comment on "High-Accuracy Estimation of "Slow" Molecular Diffusion Rates in Zeolite Nanopores, Based on Free Energy Calculations at an Ultrahigh Temperature". <i>Journal of Physical Chemistry C</i> , 2008, 112, 17030-17031.	1.5	6
104	Effect of pressure on the ionic conductivity of Li ⁺ and Cl ⁻ ions in water. <i>Journal of Chemical Physics</i> , 2012, 137, 144506.	1.2	6
105	Mean-field results of a lattice-gas model of multilayer adsorption. <i>Chemical Physics Letters</i> , 1984, 110, 265-269.	1.2	5
106	Glass transition in isopentane: A Monte Carlo study. <i>Physical Review B</i> , 1985, 31, 3196-3198.	1.1	5
107	Dynamics of propane in Na-Y zeolite. <i>Applied Physics A: Materials Science and Processing</i> , 2002, 74, s1317-s1319.	1.1	5
108	Organization of Copper Azide Clusters into Two-Dimensional Structures: Synthesis, Structure, and Magnetic Properties. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 2173-2183.	1.0	5

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109	Understanding fast diffusion of solutes in solid solutions: A molecular dynamics study of solutes in body centered cubic solid. <i>Journal of Chemical Physics</i> , 2020, 153, 244503.	1.2	5
110	Study of adsorbed molecules by Auger spectroscopy. <i>Applications of Surface Science</i> , 1982, 10, 559-566.	1.0	4
111	Sorbate Properties of Xenon in Cloverite: A Molecular Dynamics Study. <i>Journal of Solid State Chemistry</i> , 1994, 111, 151-156.	1.4	4
112	A Monte Carlo Method for Estimation of Pore Volumes of Zeolites. <i>Zeolites</i> , 1997, 19, 51-56.	0.9	4
113	A study of the condensed phases and solid-solid phase transition in toluene: A Monte Carlo investigation. <i>Journal of Chemical Physics</i> , 2000, 113, 8070-8079.	1.2	4
114	Diffusion of hydrocarbons in confined media: Translational and rotational motion. <i>Journal of Chemical Sciences</i> , 2001, 113, 559-577.	0.7	4
115	Source of Reaction-Diffusion Coupling in Confined Systems due to Temperature Inhomogeneities. <i>Physical Review Letters</i> , 2002, 88, 120601.	2.9	4
116	Levitation effect: Size-dependent maximum in rotational diffusion in confined systems. <i>Journal of Chemical Physics</i> , 2005, 122, 144505.	1.2	4
117	Separation of Mixtures at Nano Length Scales: A Blow Torch and Levitation Effect. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3835-3840.	1.2	4
118	Structure, energetics and diffusion properties of isomers of trimethyl benzene in $\hat{1}^2$ zeolite: Uptake and Monte Carlo simulation study. <i>Microporous and Mesoporous Materials</i> , 2009, 125, 135-142.	2.2	4
119	Understanding Translational-Rotational Coupling in Liquid Water through Changes in Mass Distribution. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11344-11355.	1.2	4
120	Shared hydrogen bonds: water in aluminated faujasite. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 1632-1639.	1.3	4
121	New methods of probing the structure of catalysts. <i>International Reviews in Physical Chemistry</i> , 1988, 7, 81-87.	0.9	3
122	Effect of Sorbate-Zeolite Interaction on Cluster Lifetime and Size of Sorbates: Xe in NaY. <i>Journal of Solid State Chemistry</i> , 1993, 106, 184-189.	1.4	3
123	Monte Carlo simulation of an argon cluster confined in zeolite NaCaA. <i>Chemical Physics Letters</i> , 1996, 252, 384-388.	1.2	3
124	Classification of the third regime in the size dependence of self diffusivity in levitation effect. <i>Chemical Physics Letters</i> , 2005, 402, 222-226.	1.2	3
125	Effect of Pressure on Pedal Motion in Stilbene Molecular Crystals and Its Dependence on the Crystallographic Site. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12107-12114.	1.2	3
126	A new empirical potential for zeolite with variable Si/Al ratio: Simulations vs. experiments. <i>Microporous and Mesoporous Materials</i> , 2020, 300, 110119.	2.2	3

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127	High purity separation of n-pentane from neopentane using a nano-crystal of zeolite Y. Journal of Chemical Physics, 2021, 155, 014702.	1.2	3
128	Advances in the characterization of catalysts. Reaction Kinetics and Catalysis Letters, 1987, 35, 249-259.	0.6	2
129	Deviation from Arrhenius behaviour of rate of intercage diffusion in Zeolite Y ¹ , 1996, 1, 87-92.		2
130	Variation of diffusivity with the cation radii in molten salts of superionic conductors containing iodine anion: A molecular dynamics study. Journal of Chemical Sciences, 2012, 124, 159-166.	0.7	2
131	Structure and dynamics of cumene and 1,2,4-trimethylbenzene mixture in NaY zeolite: a molecular dynamics simulation study. Molecular Simulation, 2015, 41, 423-431.	0.9	2
132	Comparison of positional disorder in the liquid and glassy states of hydrocarbons: Dependence of disorder on molecular shape. Molecular Physics, 1994, 81, 467-473.	0.8	1
133	Low temperature intracage and intercage migration rates for guest atoms of varying sizes in zeolite NaY. Chemical Physics Letters, 2002, 359, 507-515.	1.2	1
134	Influence of temperature inhomogeneity on product profile of reactions occurring within zeolites. Journal of Chemical Sciences, 2003, 115, 543-552.	0.7	1
135	Dependence of self-diffusivity on size of impurity atoms in a face-centred cubic solid: existence of an anomalous maximum. Molecular Simulation, 2009, 35, 151-161.	0.9	1
136	How does contrasting dependence of impurity-atom diffusivity on the density of host disordered medium arise?. Indian Journal of Physics, 2009, 83, 31-47.	0.9	1
137	Levitation Effect: Role of Symmetry and Dependence of Diffusivity on the Bond Length of Homonuclear and Heteronuclear Diatomic Species. Journal of Physical Chemistry B, 2011, 115, 3514-3521.	1.2	1
138	A molecular dynamics calculation of solid phase of malonic acid: role of hydrogen-bond chains and the elastic constants. Journal of Chemical Sciences, 2017, 129, 963-974.	0.7	1
139	Separating a linear C ₅ hydrocarbon from a branched C ₆ hydrocarbon: n-pentane from 2,2-dimethyl butane using levitation and blow torch effects. Physical Chemistry Chemical Physics, 2021, 23, 18102-18111.	1.3	1
140	Mutual Diffusivity of an n-Hexane-2,2-Dimethyl Butane Binary Mixture Confined to Zeolite Y. Journal of Physical Chemistry B, 2020, 124, 8618-8627.	1.2	1
141	Effect of confinement in the $\hat{\pm}$ -cages of zeolite NaCaA on the properties of Ar ₁₃ cluster: A Monte Carlo study. Journal of Chemical Sciences, 1997, 109, 189-202.	0.7	1
142	Role of molecular reorientation in the vitrification of molecular liquids: A Monte Carlo study of the liquid and glassy states of 2,2-dimethylbutane. Journal of Molecular Liquids, 1993, 57, 177-193.	2.3	0
143	Influence of the Methane-Zeolite Interaction Potential on the Concentration Dependence of Self-Diffusivity. Adsorption Science and Technology, 2011, 29, 553-567.	1.5	0
144	Orientalional glassy phases of C ₆₀ and neopentane.: A Monte Carlo study. World Scientific Series in 20th Century Chemistry, 1995, , 258-262.	0.0	0

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145	Comparison of positional disorder in the liquid and glassy states of hydrocarbons: dependence of disorder on molecular shape. World Scientific Series in 20th Century Chemistry, 1995, , 263-269.	0.0	0
146	Computer Simulation of Transformations in Solids. World Scientific Series in 20th Century Chemistry, 1995, , 237-257.	0.0	0
147	10.1063/1.4981257.1. , 2017, , .		0
148	Separation of hydrocarbon mixture of neopentane and <i>n</i> -hexane using NaY zeolite: Large distinct diffusivity. Journal of Computational Chemistry, 2022, 43, 660-673.	1.5	0
149	Kinetic Separation of <i>n</i> -Hexane from 2,2-Dimethyl Butane in Zeolite Y Using the Novel Levi-Blow Method. Advanced Theory and Simulations, 2022, 5, 2100204.	1.3	0