Saman Alavi

List of Publications by Year
in descending order

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163 papers	6,826 citations	61984 43 h-index	74163 75 g-index
200 all docs	200 docs citations	200 times ranked	5443 citing authors

#	Article	IF	Citations
1	Direct Observation and Quantification of CO ₂ Binding Within an Amine-Functionalized Nanoporous Solid. Science, 2010, 330, 650-653.	12.6	860
2	Water proton configurations in structures I, II, and H clathrate hydrate unit cells. Journal of Chemical Physics, 2013, 138, 124504.	3.0	193
3	Molecular Dynamics Simulations of the Melting of Aluminum Nanoparticlesâ€. Journal of Physical Chemistry A, 2006, 110, 1518-1523.	2.5	182
4	Molecular dynamics simulation of imidazolium-based ionic liquids. I. Dynamics and diffusion coefficient. Journal of Chemical Physics, 2008, 129, 224508.	3.0	176
5	Molecular-dynamics study of structure II hydrogen clathrates. Journal of Chemical Physics, 2005, 123, 024507.	3.0	162
6	Linking microscopic guest properties to macroscopic observables in clathrate hydrates: Guest-host hydrogen bonding. Journal of Chemical Physics, 2009, 130, 174501.	3.0	141
7	Competition and Cooperativity in Carbon Dioxide Sorption by Amineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 1826-1829.	13.8	131
8	Effect of Guestâ€“Host Hydrogen Bonding on the Structures and Properties of Clathrate Hydrates. Chemistry - A European Journal, 2010, 16, 1017-1025.	3.3	121
9	Methanol incorporation in clathrate hydrates and the implications for oil and gas pipeline flow assurance and icy planetary bodies. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8437-8442.	7.1	113
10	Inducing Desorption of Organic Molecules with a Scanning Tunneling Microscope: Theory and Experiments. Physical Review Letters, 2000, 85, 5372-5375.	7.8	112
11	Some current challenges in clathrate hydrate science: Nucleation, decomposition and the memory effect. Current Opinion in Solid State and Materials Science, 2016, 20, 344-351.	11.5	112
12	Hydrogen-bonding alcohol-water interactions in binary ethanol, 1-propanol, and 2-propanol+methane structure II clathrate hydrates. Journal of Chemical Physics, 2010, 133, 074505.	3.0	110
13	Hydrogen-Gas Migration through Clathrate Hydrate Cages. Angewandte Chemie - International Edition, 2007, 46, 6102-6105.	13.8	109
14	Formation of methane nano-bubbles during hydrate decomposition and their effect on hydrate growth. Journal of Chemical Physics, 2015, 142, 214701.	3.0	103
15	Molecular-dynamics simulations of binary structure II hydrogen and tetrahydrofurane clathrates. Journal of Chemical Physics, 2006, 124, 014704.	3.0	100
16	Ammonia clathrate hydrates as new solid phases for Titan, Enceladus, and other planetary systems. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 14785-14790.	7.1	99
17	Molecular Modeling of the Dissociation of Methane Hydrate in Contact with a Silica Surface. Journal of Physical Chemistry B, 2012, 116, 3188-3197.	2.6	92
18	Nonequilibrium adiabatic molecular dynamics simulations of methane clathrate hydrate decomposition. Journal of Chemical Physics, 2010, 132, 144703.	3.0	91

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19	Molecular dynamics studies of melting and some liquid-state properties of 1-ethyl-3-methylimidazolium hexafluorophosphate [emim][PF6]. Journal of Chemical Physics, 2005, 122, 154704.	3.0	90
20	Simulations of structural and dynamic anisotropy in nano-confined water between parallel graphite plates. Journal of Chemical Physics, 2012, 137, 184703.	3.0	84
21	Why ice-binding type I antifreeze protein acts as a gas hydrate crystal inhibitor. Physical Chemistry Chemical Physics, 2015, 17, 9984-9990.	2.8	84
22	Grand-Canonical Monte Carlo and Molecular-Dynamics Simulations of Carbon-Dioxide and Carbon-Monoxide Adsorption in Zeolitic Imidazolate Framework Materials. Journal of Physical Chemistry C, 2010, 114, 2171-2178.	3.1	83
23	Molecular simulation of non-equilibrium methane hydrate decomposition process. Journal of Chemical Thermodynamics, 2012, 44, 13-19.	2.0	79
24	Molecular dynamics simulation of imidazolium-based ionic liquids. II. Transport coefficients. Journal of Chemical Physics, 2009, 130, 014703.	3.0	76
25	Free energies of carbon dioxide sequestration and methane recovery in clathrate hydrates. Journal of Chemical Physics, 2007, 127, 124510.	3.0	75
26	Evolution of methane during gas hydrate dissociation. Fluid Phase Equilibria, 2013, 358, 114-120.	2.5	75
27	Tuning methane content in gas hydrates via thermodynamic modeling and molecular dynamics simulation. Fluid Phase Equilibria, 2008, 263, 6-17.	2.5	70
28	Antifreeze proteins as gas hydrate inhibitors. Canadian Journal of Chemistry, 2015, 93, 839-849.	1.1	68
29	Guest-Host Hydrogen Bonding in Structure H Clathrate Hydrates. ChemPhysChem, 2009, 10, 824-829.	2.1	65
30	Effect of small cage guests on hydrogen bonding of tetrahydrofuran in binary structure II clathrate hydrates. Journal of Chemical Physics, 2012, 137, 054712.	3.0	65
31	Influence of Hydrated Silica Surfaces on Interfacial Water in the Presence of Clathrate Hydrate Forming Gases. Journal of Physical Chemistry C, 2012, 116, 24907-24915.	3.1	61
32	Current-triggered vibrational excitation in single-molecule transistors. Chemical Physics, 2002, 281, 293-303.	1.9	58
33	Waterâ€“Halogen Interactions in Chlorine and Bromine Clathrate Hydrates: An Example of Multidirectional Halogen Bonding. Journal of Physical Chemistry C, 2013, 117, 14176-14182.	3.1	55
34	Facilitating guest transport in clathrate hydrates by tuning guest-host interactions. Journal of Chemical Physics, 2015, 142, 074705.	3.0	52
35	Molecular dynamics studies of melting and solid-state transitions of ammonium nitrate. Journal of Chemical Physics, 2004, 120, 9151-9159.	3.0	49
36	Molecular dynamics simulations of the structure and transport properties of tetra-butylphosphonium amino acid ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 8826.	2.8	49

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37	Selective occupancy of methane by cage symmetry in TBAB ionic clathrate hydrate. Chemical Communications, 2016, 52, 5621-5624.	4.1	49
38	Communication: Single crystal x-ray diffraction observation of hydrogen bonding between 1-propanol and water in a structure II clathrate hydrate. Journal of Chemical Physics, 2011, 134, 121104.	3.0	47
39	Theoretical study of proton transfer in ammonium nitrate clusters. Journal of Chemical Physics, 2002, 117, 2599-2608.	3.0	45
40	Stability of rare gas structure H clathrate hydrates. Journal of Chemical Physics, 2006, 125, 104501.	3.0	45
41	NMR crystallography of p-tert-butylcalix[4]arene hostâ€“guest complexes using 1H complexation-induced chemical shifts. Physical Chemistry Chemical Physics, 2008, 10, 3857.	2.8	45
42	Phase Behavior and Structural Characterization of Ionic Clathrate Hydrate Formed with Tetra-n-butylphosphonium Hydroxide: Discovery of Primitive Crystal Structure. Crystal Growth and Design, 2015, 15, 3862-3867.	3.0	45
43	Toward control of surface reactions with a scanning tunneling microscope. Structure and dynamics of benzene desorption from a silicon surface. Journal of Chemical Physics, 2000, 113, 4412-4423.	3.0	44
44	Molecular dynamics Gibbs free energy calculations for CO2 capture and storage in structure I clathrate hydrates in the presence of SO2, CH4, N2, and H2S impurities. Journal of Chemical Thermodynamics, 2012, 44, 5-12.	2.0	44
45	Molecular dynamics studies of melting and liquid properties of ammonium dinitramide. Journal of Chemical Physics, 2003, 119, 6698-6708.	3.0	43
46	Surface Tensions in NaClâˆ'Waterâˆ'Air Systems from MD Simulations. Journal of Physical Chemistry B, 2007, 111, 11989-11996.	2.6	41
47	Synthesis and characterization of clathrate hydrates containing carbon dioxide and ethanol. Physical Chemistry Chemical Physics, 2010, 12, 9927.	2.8	41
48	Molecular dynamics study of the stability of methane structure H clathrate hydrates. Journal of Chemical Physics, 2007, 126, 124708.	3.0	40
49	Distortion of the Large Cages Encapsulating Cyclic Molecules and Empty Small Cages of Structure II Clathrate Hydrates. Journal of Physical Chemistry C, 2018, 122, 18134-18141.	3.1	40
50	Controlling organic reactions on silicon surfaces with a scanning tunneling microscope: Theoretical and experimental studies of resonance-mediated desorption. Faraday Discussions, 2000, 117, 213-229.	3.2	39
51	Molecular dynamics simulations of binary structure H hydrogen and methyl-tert-butylether clathrate hydrates. Journal of Chemical Physics, 2006, 124, 204707.	3.0	39
52	Thermophysical property measurements of tetrabutylphosphonium acetate (TBPAce) ionic semiclathrate hydrate as thermal energy storage medium for general air conditioning systems. International Journal of Refrigeration, 2018, 88, 102-107.	3.4	38
53	13C NMR Studies of Hydrocarbon Guests in Synthetic Structure H Gas Hydrates: Experiment and Computation. Journal of Physical Chemistry A, 2011, 115, 1650-1657.	2.5	37
54	Adsorption of HCl on Single-Crystal Î±-Al2O3(0001) Surface:Â A DFT Study. Journal of Physical Chemistry B, 2003, 107, 186-195.	2.6	36

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55	Determination of NMR Lineshape Anisotropy of Guest Molecules within Inclusion Complexes from Molecular Dynamics Simulations. ChemPhysChem, 2008, 9, 911-919.	2.1	36
56	A molecular dynamics study of ethanolâ€“water hydrogen bonding in binary structure I clathrate hydrate with CO2. Journal of Chemical Physics, 2011, 134, 054702.	3.0	36
57	Crystal engineering the clathrate hydrate lattice with NH₄F. CrystEngComm, 2014, 16, 7209-7217.	2.6	36
58	Investigation of Some Regularities for Dense Fluids Using a Simple Equation of State. The Journal of Physical Chemistry, 1995, 99, 9248-9252.	2.9	35
59	Molecular Dynamics Simulations of the Oxidation of Aluminum Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 209-214.	2.6	35
60	Molecular Dynamics Simulations of Hydrogen Bonding in Clathrate Hydrates with Ammonia and Methanol Guest Molecules. Journal of Chemical & Engineering Data, 2015, 60, 389-397.	1.9	34
61	Urea and Urea Nitrate Decomposition Pathways:Â A Quantum Chemistry Study. Journal of Physical Chemistry A, 2006, 110, 2759-2770.	2.5	33
62	Molecular Dynamics Simulations of Equilibrium and Transport Properties of Amino Acid-Based Room Temperature Ionic Liquids. Journal of Physical Chemistry B, 2009, 113, 8103-8113.	2.6	33
63	Antifreezes Act as Catalysts for Methane Hydrate Formation from Ice. Angewandte Chemie - International Edition, 2014, 53, 10429-10433.	13.8	33
64	How much carbon dioxide can be stored in the structure H clathrate hydrates?: A molecular dynamics study. Journal of Chemical Physics, 2007, 126, 044703.	3.0	31
65	Hydrogen Adsorption and Diffusion in pâ€tertâ€Butylcalix[4]arene: An Experimental and Molecular Simulation Study. Chemistry - A European Journal, 2010, 16, 11689-11696.	3.3	31
66	Effect of Guest Size and Conformation on Crystal Structure and Stability of Structure H Clathrate Hydrates: Experimental and Molecular Dynamics Simulation Studies. Journal of Physical Chemistry C, 2013, 117, 10473-10482.	3.1	31
67	Anisotropic Lattice Expansion of Structure H Clathrate Hydrates Induced by Help Guest: Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2014, 118, 21323-21330.	3.1	31
68	Simulations of the Solid, Liquid, and Melting of 1-n-Butyl-4-amino-1,2,4-triazolium Bromide. Journal of Physical Chemistry B, 2005, 109, 18127-18134.	2.6	29
69	A new expression for radial distribution function and infinite shear modulus of Lennard-Jones fluids. Chemical Physics, 2006, 325, 554-562.	1.9	29
70	Interfacial properties of hydrocarbon/water systems predicted by molecular dynamic simulations. Journal of Chemical Physics, 2019, 150, 114703.	3.0	29
71	Improvement of continuous hydrate-based CO2 separation by forming structure II hydrate in the system of H2Â+ÂCO2Â+ÂH2OÂ+ÂTetrahydropyran (THP). Fuel, 2020, 278, 118330.	6.4	29
72	Improved initial density dependence of the viscosity and a corresponding states function for high pressures. Physica A: Statistical Mechanics and Its Applications, 1998, 260, 31-48.	2.6	28

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73	Hydrogen bonding and proton transfer in small hydroxylammonium nitrate clusters: A theoretical study. Journal of Chemical Physics, 2003, 119, 4274-4282.	3.0	28
74	Simulations of melting of polyatomic solids and nanoparticles. Molecular Simulation, 2006, 32, 999-1015.	2.0	28
75	Molecular dynamics study of structure H clathrate hydrates of methane and large guest molecules. Journal of Chemical Physics, 2008, 128, 194505.	3.0	28
76	Molecular Simulations of Methane Hydrate Nucleation. ChemPhysChem, 2010, 11, 978-980.	2.1	27
77	Proton transfer in gas-phase ammonium dinitramide clusters. Journal of Chemical Physics, 2003, 118, 2599.	3.0	26
78	Molecular Dynamics Simulation Study of Adsorption and Patterning of DNA Bases on the Au(111) Surface. Journal of Physical Chemistry C, 2011, 115, 22484-22494.	3.1	26
79	Void-induced dissolution in molecular dynamics simulations of NaCl and water. Journal of Chemical Physics, 2006, 124, 154713.	3.0	25
80	Understanding decomposition and encapsulation energies of structure I and II clathrate hydrates. Journal of Chemical Physics, 2016, 145, 154708.	3.0	25
81	Simulations of hydrogen gas in clathrate hydrates. Molecular Simulation, 2017, 43, 808-820.	2.0	25
82	Decomposition pathways of dinitramic acid and the dinitramide ion. Journal of Chemical Physics, 2003, 119, 232-240.	3.0	24
83	Vertical excitation energies for ribose and deoxyribose nucleosides. Journal of Computational Chemistry, 2007, 28, 1776-1782.	3.3	24
84	Migration of hydrogen radicals through clathrate hydrate cages. Chemical Physics Letters, 2009, 479, 234-237.	2.6	24
85	A molecular dynamics study of guestâ€“host hydrogen bonding in alcohol clathrate hydrates. Physical Chemistry Chemical Physics, 2015, 17, 12639-12647.	2.8	24
86	Synthesis and characterization of a structure H hydrate formed with carbon dioxide and 3,3-dimethyl-2-butanone. Chemical Communications, 2013, 49, 505-507.	4.1	23
87	Structure and Guest Dynamics in Binary Clathrate Hydrates of Tetrahydropyran with Carbon Dioxide/Methane. Journal of Physical Chemistry C, 2015, 119, 25738-25746.	3.1	23
88	Reaction induced by a scanning tunneling microscope: Theory and application. Journal of Chemical Physics, 2001, 115, 1882-1890.	3.0	22
89	Selected thermophysical properties of dense fluids using a general regularity. International Journal of Thermophysics, 1995, 16, 1421-1428.	2.1	21
90	Prediction of the thermal conductivity of gases based on the Rainwaterâ€“Friend theory and a new corresponding states function. Physica A: Statistical Mechanics and Its Applications, 2000, 275, 48-69.	2.6	21

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91	Theoretical predictions of the decomposition mechanism of 1,3,3-trinitroazetidine (TNAZ). Journal of Chemical Physics, 2003, 119, 8297-8304.	3.0	21
92	Simulations of structure II H2 and D2 clathrates: Potentials incorporating quantum corrections. Journal of Chemical Physics, 2008, 128, 064506.	3.0	21
93	Molecular Dynamics Simulations ofp-tert-Butylcalix[4]arene with Small Guest Molecules. Chemistry - A European Journal, 2006, 12, 5231-5237.	3.3	20
94	A double quantum 129Xe NMR experiment for probing xenon in multiply-occupied cavities of solid-state inclusion compounds. Physical Chemistry Chemical Physics, 2007, 9, 1093.	2.8	20
95	Interactions between Structure H Hydrate Formers and Water Molecules. Journal of Physical Chemistry C, 2008, 112, 9106-9113.	3.1	20
96	Molecular dynamics simulation of 13C NMR powder lineshapes of CO in structure I clathrate hydrate. Physical Chemistry Chemical Physics, 2009, 11, 8821.	2.8	20
97	Molecular Dynamics and ab Initio Studies of the Effects of Substituent Groups on the Thermodynamic Properties and Structure of Four Selected Imidazolium-Based [Tf₂N^{â€“}] Ionic Liquids. Journal of Chemical & Engineering Data, 2014, 59, 2834-2849.	1.9	20
98	Quantum chemical study of biradical decay channels in cytidine nucleosides. Chemical Physics Letters, 2006, 426, 398-404.	2.6	18
99	Inter-cage dynamics in structure I, II, and H fluoromethane hydrates as studied by NMR and molecular dynamics simulations. Journal of Chemical Physics, 2014, 140, 214703.	3.0	18
100	Molecular dynamics simulations of interfacial properties of the CO2â€“water and CO2â€“CH4â€“water systems. Journal of Chemical Physics, 2020, 153, 044701.	3.0	18
101	NMR shielding constants for hydrogen guest molecules in structure II clathrates. Journal of Chemical Physics, 2005, 123, 051107.	3.0	17
102	Theoretical predictions of the initial decomposition steps of dimethylnitramine. Journal of Chemical Physics, 2005, 123, 074313.	3.0	17
103	Phase Transition of a Structureâ€…II Cubic Clathrate Hydrate to a Tetragonal Form. Angewandte Chemie - International Edition, 2016, 55, 9287-9291.	13.8	17
104	Computational approaches and sigma-hole interactions: general discussion. Faraday Discussions, 2017, 203, 131-163.	3.2	17
105	Thermodynamic Stability of Structure H Hydrates Based on the Molecular Properties of Large Guest Molecules. Energies, 2012, 5, 459-465.	3.1	16
106	Thermophysical Property Measurements of Tetrabutylphosphonium Oxalate (TBPOx) Ionic Semiclathrate Hydrate as a Media for the Thermal Energy Storage System. Frontiers in Chemistry, 2020, 8, 547.	3.6	16
107	Simulations of pâ€tertâ€Butylcalix[4]arene with Multiple Occupancies of Small Guest Molecules. Chemistry - A European Journal, 2008, 14, 1965-1971.	3.3	15
108	Molecular dynamics simulation of halogen bonding in Cl₂, BrCl, and mixed Cl₂/Br₂ clathrate hydrates. Canadian Journal of Chemistry, 2015, 93, 864-873.	1.1	15

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109	A molecular-dynamics study of structural and physical properties of nitromethane nanoparticles. Journal of Chemical Physics, 2004, 120, 10231-10239.	3.0	14
110	Effect of nitrogen atom substitution in cyclic guests on properties of structure H clathrate hydrates. Canadian Journal of Chemistry, 2015, 93, 906-912.	1.1	14
111	The anomalous halogen bonding interactions between chlorine and bromine with water in clathrate hydrates. Faraday Discussions, 2017, 203, 61-77.	3.2	14
112	Molecular simulations and density functional theory calculations of bromine in clathrate hydrate phases. Journal of Chemical Physics, 2016, 144, 044501.	3.0	13
113	Molecular dynamics study of congruent melting of the equimolar ionic liquid-benzene inclusion crystal [emim][NTf2]â€¢C6H6. Journal of Chemical Physics, 2010, 132, 044507.	3.0	12
114	Diversity in Crystal Growth Dynamics and Crystal Morphology of Structure-H Hydrate. Crystal Growth and Design, 2019, 19, 6398-6404.	3.0	12
115	Equal reaction rates for all recombination pathways. Journal of Chemical Physics, 1997, 106, 1463-1466.	3.0	11
116	Effects of Alkyl-Group Substitution on the Proton-Transfer Barriers in Ammonium and Hydroxylammonium Nitrate Saltsâ€. Journal of Physical Chemistry A, 2004, 108, 8801-8809.	2.5	11
117	Molecular dynamics simulation of NMR powder lineshapes of linear guests in structure I clathrate hydrates. Physical Chemistry Chemical Physics, 2011, 13, 2367-2377.	2.8	11
118	Crystal Growth of Clathrate Hydrate with Ozone: Implication for Ozone Preservation. ACS Sustainable Chemistry and Engineering, 2020, 8, 15678-15684.	6.7	11
119	Improving thermal efficiency of hydrate-based heat engine generating renewable energy from low-grade heat sources using a crystal engineering approach. Energy, 2020, 198, 117403.	8.8	11
120	Diffusion of benzene through the beta zeolite phase. Microporous and Mesoporous Materials, 2013, 181, 29-37.	4.4	10
121	Redox potential tuning by redox-inactive anions in copper(II) complexes of non-innocent o-aminophenol-based ligand containing benzoxazole: Learning from nature. Polyhedron, 2017, 122, 219-227.	2.2	10
122	Characterization of the Clathrate Hydrate Formed with Fluoromethane and Pinacolone: The Thermodynamic Stability and Volumetric Behavior of the Structure H Binary Hydrate. Journal of Physical Chemistry B, 2021, 125, 328-337.	2.6	10
123	Structural CO₂ capture preference of semiclathrate hydrate formed with tetra-n-butylammonium chloride. CrystEngComm, 2022, 24, 4366-4371.	2.6	10
124	Preservation of carbon dioxide clathrate hydrate in the presence of fructose or glucose and absence of sugars under freezer conditions. Journal of Industrial and Engineering Chemistry, 2017, 54, 332-340.	5.8	9
125	Molecular Dynamics Study of Guestâ€“Host Hydrogen Bonding in Ethylene Oxide, Trimethylene Oxide, and Formaldehyde Structure I Clathrate Hydrates. Journal of Physical Chemistry C, 2017, 121, 8832-8840.	3.1	9
126	Molecular Dynamic Simulations of Clathrate Hydrate Anomalous Preservation: The Effect of Coating Clathrate Hydrate Phases. Journal of Physical Chemistry C, 2019, 123, 28715-28725.	3.1	9

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127	Low-Temperature Thermodynamic Study of the Metastable Empty Clathrate Hydrates Using Molecular Simulations. ACS Earth and Space Chemistry, 2019, 3, 789-799.	2.7	9
128	Selective Guest Docking in Metalâ€Organic Framework Materials. ChemPhysChem, 2010, 11, 55-57.	2.1	8
129	Physical Properties and Characterization of the Binary Clathrate Hydrate with Methane + 1,1,1,3,3-Pentafluoropropane (HFC-245fa) + Water. Journal of Physical Chemistry C, 2020, 124, 20736-20745.	3.1	7
130	Application of the linear isotherm regularity to selected fluid systems. International Journal of Thermophysics, 1997, 18, 1035-1049.	2.1	6
131	Chain relations of reduced distribution functions and their associated correlation functions. Journal of Chemical Physics, 1998, 108, 706-714.	3.0	6
132	A theoretical expression for drying time of thin lumber. Bioresource Technology, 2006, 97, 1572-1577.	9.6	6
133	Effect of Nonspherical Encapsulated Guests on the Volumetric Behavior of Structure H Clathrate Hydrates. Journal of Physical Chemistry C, 2018, 122, 27631-27639.	3.1	6
134	Molecular dynamics simulations of nano-confined methanol and methanol-water mixtures between infinite graphite plates: Structure and dynamics. Journal of Chemical Physics, 2019, 150, 144510.	3.0	6
135	Effect of Help-Guest Size and Hydrogen Bonding on the Stability of N-Methylpiperidine Structure H Clathrate Hydrate. Journal of Physical Chemistry C, 2020, 124, 5978-5986.	3.1	6
136	Methane Clathrate Formation is Catalyzed and Kinetically Inhibited by the Same Molecule: Two Facets of Methanol. Journal of Physical Chemistry B, 2021, 125, 4162-4168.	2.6	6
137	Characterization of clathrate hydrate formed in H2Â+ÂCO2Â+ÂtetrahydropyranÂ+Âwater system as carbon capture materials. Fuel, 2021, 295, 120593.	6.4	6
138	Crystal Growth of Structure-H Hydrate with Water-Soluble Large Molecule Guest Compound: 1-Methylpiperidine as a Case Study. Crystal Growth and Design, 2021, 21, 1351-1357.	3.0	6
139	Theoretical and Computational Studies of Energetic Salts. , 2005, , 431-471.		5
140	Simple Ethers as Models of Sugar Molecules in Calculations of Vertical Excitation Energies of DNA and RNA Nucleosides. Journal of Physical Chemistry A, 2005, 109, 9536-9541.	2.5	5
141	Phase Transition of a Structureâ€…II Cubic Clathrate Hydrate to a Tetragonal Form. Angewandte Chemie, 2016, 128, 9433-9437.	2.0	5
142	Interfacial tension between decane saturated with methane and water from 283.2 K to 298.2 K under pressures upto 10â€‰MPa. Journal of Industrial and Engineering Chemistry, 2020, 81, 360-366.	5.8	5
143	Managing hydrogen bonding in the clathrate hydrate of the 1-pentanol guest molecule. CrystEngComm, 2021, 23, 4708-4716.	2.6	5
144	Incorporation of Ammonium Fluoride and Methanol in Carbon Dioxide Clathrate Hydrates and Their Significance for Hydrate-Based Gas Separation. Industrial & Engineering Chemistry Research, 2021, 60, 11267-11276.	3.7	5

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145	Complete binary collision approximation for the gas transport coefficients via the time correlation formulation. Journal of Chemical Physics, 1998, 109, 3452-3460.	3.0	4
146	High-Frequency Shear Modulus and Relaxation Time of Soft-Sphere and Lennardâ€“Jones Fluids. International Journal of Thermophysics, 2004, 25, 1747-1762.	2.1	4
147	Tetrabromocatecholato Mn(III) complexes of bis(phenol) diamine ligands as models for enzymeâ€“substrate adducts of catechol dioxygenases. Polyhedron, 2016, 118, 171-179.	2.2	4
148	Stability and characterization of the structure II binary clathrate hydrate of the refrigerant trans-1,3,3,3-tetrafluoropropene + methane. New Journal of Chemistry, 2019, 43, 13068-13074.	2.8	3
149	Pinacol hydrate as a novel thermal energy storage medium for electric vehicles. Journal of Energy Storage, 2022, 51, 104404.	8.1	3
150	Moderately dense gas transport coefficients via time correlation functions. I. General formalism. Journal of Chemical Physics, 1999, 111, 6909-6921.	3.0	2
151	Bound-free gas transport coefficients via the time correlation formulation based on an atomic picture. Journal of Chemical Physics, 1999, 110, 8533-8542.	3.0	2
152	Computational prediction of temperature dependence of 13C NMR lineshapes of planar molecules in structure I clathrate hydrates. Journal of the Iranian Chemical Society, 2013, 10, 659-667.	2.2	2
153	Beyond the halogen bond: general discussion. Faraday Discussions, 2017, 203, 227-244.	3.2	2
154	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	3.2	2
155	Structural Characterization of Pyrrolidineâ€“Including Structure II Clathrate Hydrates. Crystal Growth and Design, 2021, 21, 2828-2836.	3.0	2
156	Comment on â€œCage occupancy of methane clathrate hydrates in the ternary H₂Oâ€“NH₃â€“CH₄ systemâ€• by C. Petuya, M. Choukroun, T. H. Vu, A. Desmedt, A. G. Davies, and C. Sotin, Chem. Commun., 2020, 56, 12391. Chemical Communications, 2022, 58, 4095-4098.	4.1	2
157	Effect of Methanol Guests on Thermal Properties of NH₄F-Doped THF Clathrate Hydrate. Energy & Fuels, 2022, 36, 10504-10511.	5.1	2
158	Moderately dense gas transport coefficients via time correlation functions. II. Shear viscosity and thermal conductivity. Journal of Chemical Physics, 1999, 111, 6922-6931.	3.0	1
159	Investigation of the density dependence of the shear relaxation time of dense fluids. Canadian Journal of Chemistry, 2005, 83, 236-243.	1.1	1
160	Hydrogen-Gas Migration through Clathrate Hydrate Cages. Angewandte Chemie - International Edition, 2007, 46, 8933-8933.	13.8	1
161	Proton exchange in acidâ€“base complexes induced by reaction coordinates with heavy atom motions. Chemical Physics, 2012, 402, 105-112.	1.9	1
162	Measurement and analysis of interfacial tension of decane/water system pressurized with methane + ethane + propane gas mixture. Journal of Natural Gas Science and Engineering, 2021, 96, 104333.	4.4	1

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163	Molecular Dynamics Studies of Nanoparticles of Energetic Materials. Materials Research Society Symposia Proceedings, 2003, 800, 319.	0.1	0