Saman Alavi

List of Publications by Year
in descending order

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	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
2	Pinacol hydrate as a novel thermal energy storage medium for electric vehicles. Journal of Energy Storage, 2022, 51, 104404.	8.1	3
3	Structural CO₂ capture preference of semiclathrate hydrate formed with tetra-n-butylammonium chloride. CrystEngComm, 2022, 24, 4366-4371.	2.6	10
4	Effect of Methanol Guests on Thermal Properties of NH₄F-Doped THF Clathrate Hydrate. Energy & Fuels, 2022, 36, 10504-10511.	5.1	2
5	Managing hydrogen bonding in the clathrate hydrate of the 1-pentanol guest molecule. CrystEngComm, 2021, 23, 4708-4716.	2.6	5
6	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
7	Structural Characterization of Pyrrolidineâ€“Including Structure II Clathrate Hydrates. Crystal Growth and Design, 2021, 21, 2828-2836.	3.0	2
8	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
9	Characterization of clathrate hydrate formed in H2Â+ÂCO2Â+Âtetrahydropyranâ+Âwater system as carbon capture materials. Fuel, 2021, 295, 120593.	6.4	6
10	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
11	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
12	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
13	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
14	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
15	Crystal Growth of Clathrate Hydrate with Ozone: Implication for Ozone Preservation. ACS Sustainable Chemistry and Engineering, 2020, 8, 15678-15684.	6.7	11
16	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
17	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
18	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

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19	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
20	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
21	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
22	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
23	Diversity in Crystal Growth Dynamics and Crystal Morphology of Structure-H Hydrate. Crystal Growth and Design, 2019, 19, 6398-6404.	3.0	12
24	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
25	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
26	Interfacial properties of hydrocarbon/water systems predicted by molecular dynamic simulations. Journal of Chemical Physics, 2019, 150, 114703.	3.0	29
27	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
28	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
29	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
30	Simulations of hydrogen gas in clathrate hydrates. Molecular Simulation, 2017, 43, 808-820.	2.0	25
31	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
32	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
33	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
34	Computational approaches and sigma-hole interactions: general discussion. Faraday Discussions, 2017, 203, 131-163.	3.2	17
35	Beyond the halogen bond: general discussion. Faraday Discussions, 2017, 203, 227-244.	3.2	2
36	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	3.2	2

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37	The anomalous halogen bonding interactions between chlorine and bromine with water in clathrate hydrates. Faraday Discussions, 2017, 203, 61-77.	3.2	14
38	Understanding decomposition and encapsulation energies of structure I and II clathrate hydrates. Journal of Chemical Physics, 2016, 145, 154708.	3.0	25
39	Molecular simulations and density functional theory calculations of bromine in clathrate hydrate phases. Journal of Chemical Physics, 2016, 144, 044501.	3.0	13
40	Selective occupancy of methane by cage symmetry in TBAB ionic clathrate hydrate. Chemical Communications, 2016, 52, 5621-5624.	4.1	49
41	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
42	Phase Transition of a Structureâ€…II Cubic Clathrate Hydrate to a Tetragonal Form. Angewandte Chemie, 2016, 128, 9433-9437.	2.0	5
43	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
44	Phase Transition of a Structureâ€…II Cubic Clathrate Hydrate to a Tetragonal Form. Angewandte Chemie - International Edition, 2016, 55, 9287-9291.	13.8	17
45	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
46	Antifreeze proteins as gas hydrate inhibitors. Canadian Journal of Chemistry, 2015, 93, 839-849.	1.1	68
47	Formation of methane nano-bubbles during hydrate decomposition and their effect on hydrate growth. Journal of Chemical Physics, 2015, 142, 214701.	3.0	103
48	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
49	A molecular dynamics study of guestâ€“host hydrogen bonding in alcohol clathrate hydrates. Physical Chemistry Chemical Physics, 2015, 17, 12639-12647.	2.8	24
50	Facilitating guest transport in clathrate hydrates by tuning guest-host interactions. Journal of Chemical Physics, 2015, 142, 074705.	3.0	52
51	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
52	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
53	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
54	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

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55	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
56	Antifreezes Act as Catalysts for Methane Hydrate Formation from Ice. Angewandte Chemie - International Edition, 2014, 53, 10429-10433.	13.8	33
57	Crystal engineering the clathrate hydrate lattice with NH₄F. CrystEngComm, 2014, 16, 7209-7217.	2.6	36
58	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
59	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
60	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
61	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
62	Diffusion of benzene through the beta zeolite phase. Microporous and Mesoporous Materials, 2013, 181, 29-37.	4.4	10
63	Evolution of methane during gas hydrate dissociation. Fluid Phase Equilibria, 2013, 358, 114-120.	2.5	75
64	Water proton configurations in structures I, II, and H clathrate hydrate unit cells. Journal of Chemical Physics, 2013, 138, 124504.	3.0	193
65	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
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	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
68	Thermodynamic Stability of Structure H Hydrates Based on the Molecular Properties of Large Guest Molecules. Energies, 2012, 5, 459-465.	3.1	16
69	Simulations of structural and dynamic anisotropy in nano-confined water between parallel graphite plates. Journal of Chemical Physics, 2012, 137, 184703.	3.0	84
70	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
71	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
72	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

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73	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
74	Proton exchange in acidâ€"base complexes induced by reaction coordinates with heavy atom motions. Chemical Physics, 2012, 402, 105-112.	1.9	1
75	Molecular simulation of non-equilibrium methane hydrate decomposition process. Journal of Chemical Thermodynamics, 2012, 44, 13-19.	2.0	79
76	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
77	Competition and Cooperativity in Carbon Dioxide Sorption by Amineâ€Functionalized Metalâ€"Organic Frameworks. Angewandte Chemie - International Edition, 2012, 51, 1826-1829.	13.8	131
78	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
79	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
80	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
81	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
82	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
83	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
84	Synthesis and characterization of clathrate hydrates containing carbon dioxide and ethanol. Physical Chemistry Chemical Physics, 2010, 12, 9927.	2.8	41
85	Selective Guest Docking in Metalâ€Organic Framework Materials. ChemPhysChem, 2010, 11, 55-57.	2.1	8
86	Molecular Simulations of Methane Hydrate Nucleation. ChemPhysChem, 2010, 11, 978-980.	2.1	27
87	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
88	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
89	Nonequilibrium adiabatic molecular dynamics simulations of methane clathrate hydrate decomposition. Journal of Chemical Physics, 2010, 132, 144703.	3.0	91
90	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

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91	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
92	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
93	Direct Observation and Quantification of CO ₂ Binding Within an Amine-Functionalized Nanoporous Solid. Science, 2010, 330, 650-653.	12.6	860
94	Molecular dynamics simulation of imidazolium-based ionic liquids. II. Transport coefficients. Journal of Chemical Physics, 2009, 130, 014703.	3.0	76
95	Guest-Host Hydrogen Bonding in Structure H Clathrate Hydrates. ChemPhysChem, 2009, 10, 824-829.	2.1	65
96	Migration of hydrogen radicals through clathrate hydrate cages. Chemical Physics Letters, 2009, 479, 234-237.	2.6	24
97	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
98	Linking microscopic guest properties to macroscopic observables in clathrate hydrates: Guest-host hydrogen bonding. Journal of Chemical Physics, 2009, 130, 174501.	3.0	141
99	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
100	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
101	Determination of NMR Lineshape Anisotropy of Guest Molecules within Inclusion Complexes from Molecular Dynamics Simulations. ChemPhysChem, 2008, 9, 911-919.	2.1	36
102	Tuning methane content in gas hydrates via thermodynamic modeling and molecular dynamics simulation. Fluid Phase Equilibria, 2008, 263, 6-17.	2.5	70
103	Molecular dynamics simulation of imidazolium-based ionic liquids. I. Dynamics and diffusion coefficient. Journal of Chemical Physics, 2008, 129, 224508.	3.0	176
104	Interactions between Structure H Hydrate Formers and Water Molecules. Journal of Physical Chemistry C, 2008, 112, 9106-9113.	3.1	20
105	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
106	Molecular dynamics study of structure H clathrate hydrates of methane and large guest molecules. Journal of Chemical Physics, 2008, 128, 194505.	3.0	28
107	Simulations of structure II H2 and D2 clathrates: Potentials incorporating quantum corrections. Journal of Chemical Physics, 2008, 128, 064506.	3.0	21
108	Free energies of carbon dioxide sequestration and methane recovery in clathrate hydrates. Journal of Chemical Physics, 2007, 127, 124510.	3.0	75

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109	Molecular dynamics study of the stability of methane structure H clathrate hydrates. Journal of Chemical Physics, 2007, 126, 124708.	3.0	40
110	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
111	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
112	Surface Tensions in NaClâˆ'Waterâˆ'Air Systems from MD Simulations. Journal of Physical Chemistry B, 2007, 111, 11989-11996.	2.6	41
113	Hydrogen-Gas Migration through Clathrate Hydrate Cages. Angewandte Chemie - International Edition, 2007, 46, 6102-6105.	13.8	109
114	Hydrogen-Gas Migration through Clathrate Hydrate Cages. Angewandte Chemie - International Edition, 2007, 46, 8933-8933.	13.8	1
115	Vertical excitation energies for ribose and deoxyribose nucleosides. Journal of Computational Chemistry, 2007, 28, 1776-1782.	3.3	24
116	Molecular Dynamics Simulations of the Melting of Aluminum Nanoparticlesâ€. Journal of Physical Chemistry A, 2006, 110, 1518-1523.	2.5	182
117	Void-induced dissolution in molecular dynamics simulations of NaCl and water. Journal of Chemical Physics, 2006, 124, 154713.	3.0	25
118	Simulations of melting of polyatomic solids and nanoparticles. Molecular Simulation, 2006, 32, 999-1015.	2.0	28
119	Stability of rare gas structure H clathrate hydrates. Journal of Chemical Physics, 2006, 125, 104501.	3.0	45
120	Urea and Urea Nitrate Decomposition Pathways:Â A Quantum Chemistry Study. Journal of Physical Chemistry A, 2006, 110, 2759-2770.	2.5	33
121	Molecular dynamics simulations of binary structure H hydrogen and methyl-tert-butylether clathrate hydrates. Journal of Chemical Physics, 2006, 124, 204707.	3.0	39
122	Molecular-dynamics simulations of binary structure II hydrogen and tetrahydrofurane clathrates. Journal of Chemical Physics, 2006, 124, 014704.	3.0	100
123	A theoretical expression for drying time of thin lumber. Bioresource Technology, 2006, 97, 1572-1577.	9.6	6
124	Quantum chemical study of biradical decay channels in cytidine nucleosides. Chemical Physics Letters, 2006, 426, 398-404.	2.6	18
125	A new expression for radial distribution function and infinite shear modulus of Lennard-Jones fluids. Chemical Physics, 2006, 325, 554-562.	1.9	29
126	Molecular Dynamics Simulations ofp-tert-Butylcalix[4]arene with Small Guest Molecules. Chemistry - A European Journal, 2006, 12, 5231-5237.	3.3	20

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127	Theoretical and Computational Studies of Energetic Salts. , 2005, , 431-471.		5
128	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
129	NMR shielding constants for hydrogen guest molecules in structure II clathrates. Journal of Chemical Physics, 2005, 123, 051107.	3.0	17
130	Theoretical predictions of the initial decomposition steps of dimethylnitramine. Journal of Chemical Physics, 2005, 123, 074313.	3.0	17
131	Investigation of the density dependence of the shear relaxation time of dense fluids. Canadian Journal of Chemistry, 2005, 83, 236-243.	1.1	1
132	Molecular Dynamics Simulations of the Oxidation of Aluminum Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 209-214.	2.6	35
133	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
134	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
135	Molecular-dynamics study of structure II hydrogen clathrates. Journal of Chemical Physics, 2005, 123, 024507.	3.0	162
136	Molecular dynamics studies of melting and solid-state transitions of ammonium nitrate. Journal of Chemical Physics, 2004, 120, 9151-9159.	3.0	49
137	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
138	A molecular-dynamics study of structural and physical properties of nitromethane nanoparticles. Journal of Chemical Physics, 2004, 120, 10231-10239.	3.0	14
139	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
140	Hydrogen bonding and proton transfer in small hydroxylammonium nitrate clusters: A theoretical study. Journal of Chemical Physics, 2003, 119, 4274-4282.	3.0	28
141	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
142	Proton transfer in gas-phase ammonium dinitramide clusters. Journal of Chemical Physics, 2003, 118, 2599.	3.0	26
143	Molecular Dynamics Studies of Nanoparticles of Energetic Materials. Materials Research Society Symposia Proceedings, 2003, 800, 319.	0.1	0
144	Decomposition pathways of dinitramic acid and the dinitramide ion. Journal of Chemical Physics, 2003, 119, 232-240.	3.0	24

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145	Molecular dynamics studies of melting and liquid properties of ammonium dinitramide. Journal of Chemical Physics, 2003, 119, 6698-6708.	3.0	43
146	Theoretical predictions of the decomposition mechanism of 1,3,3-trinitroazetidine (TNAZ). Journal of Chemical Physics, 2003, 119, 8297-8304.	3.0	21
147	Theoretical study of proton transfer in ammonium nitrate clusters. Journal of Chemical Physics, 2002, 117, 2599-2608.	3.0	45
148	Current-triggered vibrational excitation in single-molecule transistors. Chemical Physics, 2002, 281, 293-303.	1.9	58
149	Reaction induced by a scanning tunneling microscope: Theory and application. Journal of Chemical Physics, 2001, 115, 1882-1890.	3.0	22
150	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
151	Inducing Desorption of Organic Molecules with a Scanning Tunneling Microscope: Theory and Experiments. Physical Review Letters, 2000, 85, 5372-5375.	7.8	112
152	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
153	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
154	Moderately dense gas transport coefficients via time correlation functions. I. General formalism. Journal of Chemical Physics, 1999, 111, 6909-6921.	3.0	2
155	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
156	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
157	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
158	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
159	Chain relations of reduced distribution functions and their associated correlation functions. Journal of Chemical Physics, 1998, 108, 706-714.	3.0	6
160	Equal reaction rates for all recombination pathways. Journal of Chemical Physics, 1997, 106, 1463-1466.	3.0	11
161	Application of the linear isotherm regularity to selected fluid systems. International Journal of Thermophysics, 1997, 18, 1035-1049.	2.1	6
162	Selected thermophysical properties of dense fluids using a general regularity. International Journal of Thermophysics, 1995, 16, 1421-1428.	2.1	21

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163	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