Stability, Adsorption, and Diffusion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CH</mml:mi><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CO</mml:mi><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="bold">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Clathrate Hydrate

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Citation Report

#	Article	IF	Citations
1	Viability of Clathrate Hydrates as CO₂ Capturing Agents: A Theoretical Study. Journal of Physical Chemistry A, 2011, 115, 7633-7637.	1.1	52
2	First-principles investigation on the structural stability of methane and ethane clathrate hydrates. Computational and Theoretical Chemistry, 2011, 977, 209-212.	1.1	14
3	Ab initioenergetics and kinetics study of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and CH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>in the SI clathrate hydrate. Physical Review B, 2011, 84, .	1.1	30
4	Stability and Reactivity of Methane Clathrate Hydrates: Insights from Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 7742-7745.	1.1	55
5	Molecular vibrations of methane molecules in the structure I clathrate hydrate from ab initio molecular dynamics simulation. Journal of Chemical Physics, 2012, 136, 044508.	1.2	43
6	Titanâ€™s internal structure and the evolutionary consequences. Planetary and Space Science, 2012, 60, 10-17.	0.9	86
7	Pentagonal dodecahedron methane hydrate cage and methanol system â€” An ab initio study. Journal of Chemical Sciences, 2013, 125, 379-385.	0.7	14
8	DFT-based inhibitor and promoter selection criteria for pentagonal dodecahedron methane hydrate cage. Journal of Chemical Sciences, 2013, 125, 1259-1266.	0.7	13
9	Diffusion of Small Molecules in Metal Organic Framework Materials. Physical Review Letters, 2013, 110, 026102.	2.9	98
10	Crystal structure, stability and spectroscopic properties of methane and CO2 hydrates. Journal of Molecular Graphics and Modelling, 2013, 44, 253-265.	1.3	44
11	Adsorption of H, H2, and H2O inside and outside of (M@Si16F)6 tubelike aggregates and wires (MÂ=ÂV, Ta). A first principles study. Materials Chemistry and Physics, 2013, 139, 247-255.	2.0	3
12	Hydrocarbon Behavior at Nanoscale Interfaces. Reviews in Mineralogy and Geochemistry, 2013, 75, 495-545.	2.2	30
13	Gas Saturation Resulting from Methane Hydrate Dissociation in a Porous Medium: Comparison between Analytical and Pore-Network Results. Journal of Physical Chemistry C, 2013, 117, 11104-11116.	1.5	8
14	Prediction of Clathrate Structure Type and Guest Position by Molecular Mechanics. Journal of Physical Chemistry A, 2013, 117, 4001-4010.	1.1	31
15	Benchmarking the performance of density functional theory and point charge force fields in their description of sI methane hydrate against diffusion Monte Carlo. Journal of Chemical Physics, 2014, 140, 174703.	1.2	41
16	Density functional theoretic studies of hostâ€“guest interaction in gas hydrates. Computational and Theoretical Chemistry, 2014, 1029, 26-32.	1.1	24
17	Câ€“C Stretching Raman Spectra and Stabilities of Hydrocarbon Molecules in Natural Gas Hydrates: A Quantum Chemical Study. Journal of Physical Chemistry A, 2014, 118, 11641-11651.	1.1	27
18	Comparative investigation of polyhedral water cages of (H2O)n (n=20, 24, and 28) encaging CH4 and SF6 as guest molecules. Chemical Physics, 2014, 441, 128-136.	0.9	4

#	Article	IF	Citations
19	A quantum chemistry study of natural gas hydrates. Journal of Molecular Modeling, 2014, 20, 2182.	0.8	18
20	Molecular hydrogen solvated in water â€“ A computational study. Journal of Chemical Physics, 2015, 143, 244505.	1.2	7
21	Theoretical study of methanol as inhibitor and cyclopentane as stabilizer of dodecahedron methane hydrate cage. IOP Conference Series: Materials Science and Engineering, 2015, 73, 012081.	0.3	2
22	Guestâ€“host interactions in gas clathrate hydrates under pressure. High Pressure Research, 2015, 35, 49-56.	0.4	9
23	Design of Methane Hydrate Inhibitor Molecule Using Density Functional Theory. Journal of Cluster Science, 2015, 26, 551-563.	1.7	4
24	CH-Stretching Vibrational Trends in Natural Gas Hydrates Studied by Quantum-Chemical Computations. Journal of Physical Chemistry C, 2015, 119, 17084-17091.	1.5	20
25	A molecular dynamics study of guestâ€“host hydrogen bonding in alcohol clathrate hydrates. Physical Chemistry Chemical Physics, 2015, 17, 12639-12647.	1.3	24
26	DFT calculation of the potential energy landscape topology and Raman spectra of type I CH₄and CO₂hydrates. Physical Chemistry Chemical Physics, 2015, 17, 6963-6975.	1.3	28
27	Low barriers for hydrogen diffusion in sII clathrate. Physical Chemistry Chemical Physics, 2015, 17, 13808-13812.	1.3	34
29	Structure and stability of multiply occupied methane clathrate hydrates. Chemical Physics Letters, 2015, 637, 110-114.	1.2	11
30	Structures, Stabilities, and Spectra Properties of Fused CH₄ Endohedral Water Cage (CH₄)_m(H₂O)_n Clusters from DFT-D Methods. Journal of Physical Chemistry A, 2015, 119, 10971-10979.	1.1	10
31	In silico studies on the origin of selective uptake of carbon dioxide with cucurbit[7]uril amorphous material. RSC Advances, 2015, 5, 72469-72475.	1.7	6
32	Ab initioDFT study of structural and mechanical properties of methane and carbon dioxide hydrates. Molecular Simulation, 2015, 41, 572-579.	0.9	35
33	Replacement micro-mechanism of CH4 hydrate by N2/CO2 mixture revealed by ab initio studies. Computational Materials Science, 2016, 123, 106-110.	1.4	39
34	Molecular Mechanisms of Gas Diffusion in CO₂ Hydrates. Journal of Physical Chemistry C, 2016, 120, 16298-16304.	1.5	46
35	Polarization response of clathrate hydrates capsulated with guest molecules. Journal of Chemical Physics, 2016, 144, 204308.	1.2	11
36	Understanding decomposition and encapsulation energies of structure I and II clathrate hydrates. Journal of Chemical Physics, 2016, 145, 154708.	1.2	25
37	Understanding effect of structure and stability on transformation of CH4 hydrate to CO2 hydrate. Chemical Physics Letters, 2016, 648, 75-80.	1.2	26

#	Article	IF	Citations
38	Effect of multiple and adjacent cage occupancies on host-guest interaction and NMR chemical shifts in gas hydrates. Computational and Theoretical Chemistry, 2016, 1092, 57-67.	1.1	8
39	Theoretical investigation of exchange of N2 and H2 in sII clathrate hydrates. Chemical Physics Letters, 2016, 660, 266-271.	1.2	4
40	Chemically accurate energy barriers of small gas molecules moving through hexagonal water rings. Physical Chemistry Chemical Physics, 2016, 18, 17831-17835.	1.3	5
41	Direct transition mechanism for molecular diffusion in gas hydrates. RSC Advances, 2016, 6, 1966-1972.	1.7	25
42	Elasticity and Stability of Clathrate Hydrate: Role of Guest Molecule Motions. Scientific Reports, 2017, 7, 1290.	1.6	41
43	Water Vacancy Driven Diffusion in Clathrate Hydrates: Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2017, 121, 8280-8289.	1.5	24
44	Ab Initio Studies on the Clathrate Hydrates of Some Nitrogen- and Sulfur-Containing Gases. Journal of Physical Chemistry A, 2017, 121, 2620-2626.	1.1	16
45	Molecular mobility in carbon dioxide hydrates. Molecular Systems Design and Engineering, 2017, 2, 500-506.	1.7	7
46	The role of non-covalent interaction for the adsorption of CO₂ and hydrocarbons with per-hydroxylated pillar[6]arene: a computational study. New Journal of Chemistry, 2017, 41, 12044-12051.	1.4	32
47	Formation of clathrate cages of sI methane hydrate revealed by ab initio study. Energy, 2017, 120, 698-704.	4.5	28
48	Noncovalent Interactions in Nanotechnology. , 2017, , 417-451.		8
49	Insights into the Structure of Liquid Water from Nuclear Quantum Effects on the Density and Compressibility of Ice Polymorphs. Journal of Physical Chemistry B, 2018, 122, 5694-5706.	1.2	11
50	Formation of CO₂ Hydrates within Single-Walled Carbon Nanotubes at Ambient Pressure: CO₂ Capture and Selective Separation of a CO₂/H₂ Mixture in Water. Journal of Physical Chemistry C, 2018, 122, 7951-7958.	1.5	21
51	Hostâ€“guest and guestâ€“guest interactions in noble gas hydrates. Molecular Physics, 2018, 116, 54-63.	0.8	11
52	Simulation of Capture and Release Processes of Hydrogen by Î²-Hydroquinone Clathrate. ACS Omega, 2018, 3, 18771-18782.	1.6	16
53	A Simple Correction for Nonadditive Dispersion within Extended Symmetry-Adapted Perturbation Theory (XSAPT). Journal of Chemical Theory and Computation, 2018, 14, 5128-5142.	2.3	19
54	Prediction of efficient promoter molecules of sH hydrogen hydrate: An ab initio study. Chemical Physics, 2019, 516, 15-21.	0.9	9
55	Proton Conduction Inhibited by Xe Hydrates in the Water Nanotube of the Molecular Porous Crystal {{[Ru^{III}(H₂bim)₃](TMA)}₂Â·mH₂O}_n. Journal of Physical Chemistry C, 2019, 123, 20413-20419.	1.5	5

#	Article	IF	Citations
56	Molecular Insights into Cage Occupancy of Hydrogen Hydrate: A Computational Study. Processes, 2019, 7, 699.	1.3	11
57	Structural properties of sH hydrate: a DFT study of anisotropy and equation of state. Molecular Simulation, 2019, 45, 1524-1537.	0.9	15
58	Theoretical investigation of storage capacity of hydrocarbon gas in sH hydrate. Chemical Physics, 2019, 525, 110393.	0.9	6
59	Unraveling the metastability of the SI and SII carbon monoxide hydrate with a combined DFT-neutron diffraction investigation. Journal of Chemical Physics, 2019, 150, 184705.	1.2	12
60	Stability, Vibrations, and Diffusion of Hydrogen Gas in Clathrate Hydrates: Insights from Ab Initio Calculations on Condensed-Phase Crystalline Structures. Journal of Physical Chemistry C, 2019, 123, 12052-12061.	1.5	20
61	Phase diagram and composition of water based crystalline phases in hydrogen â€“ Water binary system. Solid State Communications, 2019, 294, 6-10.	0.9	10
62	Two-dimensional methane hydrate: Plum-pudding structure and sandwich structure. Chemical Physics Letters, 2019, 725, 38-44.	1.2	5
63	Desalination and Li+ enrichment via formation of cyclopentane hydrate. Separation and Purification Technology, 2020, 231, 115921.	3.9	29
64	Microsecond simulation study on the replacement of methane in methane hydrate by carbon dioxide, nitrogen, and carbon dioxideâ€“nitrogen mixtures. Fuel, 2020, 263, 116640.	3.4	35
65	Computational simulation of fluorinated methane derivatives in type I clathrate hydrate. Journal of Molecular Liquids, 2020, 314, 113783.	2.3	6
66	A Lattice Distortion Theory for Promotor Containing Clathrate Hydrates. Scientific Reports, 2020, 10, 9622.	1.6	2
67	Role of Methane as a Second Guest Component in Thermodynamic Stability and Isomer Selectivity of Butane Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 18474-18481.	1.5	17
68	Theoretical Characterization of the High Pressure Nonclathrate CO₂ Hydrate. ACS Earth and Space Chemistry, 2020, 4, 2121-2128.	1.2	1
69	Research progress and challenges in hydrate-based carbon dioxide capture applications. Applied Energy, 2020, 269, 114928.	5.1	88
70	Thermal decomposition and diffusion of methane in clathrate hydrates from quantum mechanics simulations. RSC Advances, 2020, 10, 14753-14760.	1.7	3
71	CH4 Gas Extraction by CO2: Substitution in Clathrate Hydrate through Bimolecular Iteration. Chinese Physics Letters, 2020, 37, 048201.	1.3	3
72	Novel methodology for the calculation of the enthalpy of enclathration of methane hydrates using molecular dynamics simulations. Molecular Physics, 2020, 118, e1711976.	0.8	1
73	Computational density-functional approaches on finite-size and guest-lattice effects in CO2@sII clathrate hydrate. Journal of Chemical Physics, 2021, 154, 044301.	1.2	10

#	Article	IF	Citations
74	Effect of Pore Geometry on Gas Adsorption: Grand Canonical Monte Carlo Simulation Studies. Bulletin of the Korean Chemical Society, 2012, 33, 901-905.	1.0	4
75	Theoretical Investigation of the Fusion Process of Mono-Cages to Tri-Cages with CH4/C2H6 Guest Molecules in sI Hydrates. Molecules, 2021, 26, 7071.	1.7	0
76	Ab initio mechanistic insights into the stability, diffusion and storage capacity of sI clathrate hydrate containing hydrogen. International Journal of Hydrogen Energy, 2022, 47, 8419-8433.	3.8	10
79	Generalized energy-based fragmentation approach for accurate binding energies and Raman spectra of methane hydrate clusters. Chinese Journal of Chemical Physics, 2022, 35, 167-176.	0.6	3
82	Carbon Capture via Ocean and Soil Separation. , 2024, , .		0