

Athanassios K Stubos

List of Publications by Year in descending order

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127
papers

5,082
citations

125106

35
h-index

111975

67
g-index

127
all docs

127
docs citations

127
times ranked

6126
citing authors

#	ARTICLE	IF	CITATIONS
1	Review on the Safe Use of Ammonia Fuel Cells in the Maritime Industry. <i>Energies</i> , 2021, 14, 3023.	1.6	46
2	Study on the operation and energy demand of dual-stage Metal Hydride Hydrogen Compressors under effective thermal management. <i>International Journal of Hydrogen Energy</i> , 2021, 46, 29272-29287.	3.8	14
3	A Practical Methodology to Estimate the H ₂ Storage Capacity of Pure and Binary Hydrates Based on Monte Carlo Simulations. <i>Journal of Chemical & Engineering Data</i> , 2020, 65, 1289-1299.	1.0	10
4	Numerical investigation on the operation and energy demand of a seven-stage metal hydride hydrogen compression system for Hydrogen Refuelling Stations. <i>Renewable Energy</i> , 2020, 147, 164-178.	4.3	19
5	Thermal characteristics of an air-cooled open-cathode proton exchange membrane fuel cell stack via numerical investigation. <i>International Journal of Energy Research</i> , 2020, 44, 11597-11613.	2.2	16
6	Recent Advances in Experimental Measurements of Mixed-Gas Three-Phase Hydrate Equilibria for Gas Mixture Separation and Energy-Related Applications. <i>Journal of Chemical & Engineering Data</i> , 2019, 64, 4991-5016.	1.0	17
7	Metal hydride hydrogen compressors: Current developments & early markets. <i>Renewable Energy</i> , 2018, 127, 850-862.	4.3	59
8	Enhanced CO ₂ selectivity within the cavity of gmelinite frameworks. <i>Adsorption</i> , 2018, 24, 371-379.	1.4	3
9	Solubility of Methane and Carbon Dioxide in the Aqueous Phase of the Ternary (Methane + Carbon Dioxide + Water) System. <i>Journal of Chemical & Engineering Data</i> , 2018, 63, 1027-1035.	1.0	15
10	Identification of conditions for increased methane storage capacity in sII and sH clathrate hydrates from Monte Carlo simulations. <i>Journal of Chemical Thermodynamics</i> , 2018, 117, 128-137.	1.0	17
11	Monte Carlo simulations of the separation of a binary gas mixture (CH ₄ + CO ₂) in clathrate hydrates. <i>Journal of Chemical Thermodynamics</i> , 2018, 117, 138-147.	1.3	17
12	Using clathrate hydrates for gas storage and gas-mixture separations: experimental and computational studies at multiple length scales. <i>Molecular Physics</i> , 2018, 116, 2041-2060.	0.8	18
13	Modeling and simulation supporting the application of fuel cell & hydrogen technologies. <i>Journal of Computational Science</i> , 2018, 27, 10-20.	1.5	6
14	Storage of H ₂ in Clathrate Hydrates: Evaluation of Different Force-Fields used in Monte Carlo Simulations. <i>Molecular Physics</i> , 2017, 115, 1274-1285.	0.8	16
15	Material development and assessment of an energy storage concept based on the CaO-looping process. <i>Solar Energy</i> , 2017, 150, 298-309.	2.9	51
16	Determining the specific surface area of Metal Organic Frameworks based on a computational approach. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2017, 526, 14-19.	2.3	2
17	Two- and three-phase equilibrium experimental measurements for the ternary CH ₄ + CO ₂ + H ₂ O mixture. <i>Fluid Phase Equilibria</i> , 2017, 451, 96-105.	1.4	15
18	The effect of lattice constant on the storage capacity of hydrogen hydrates: a Monte Carlo study. <i>Molecular Physics</i> , 2016, 114, 2664-2671.	0.8	18

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19	Lattice constants of pure methane and carbon dioxide hydrates at low temperatures. Implementing quantum corrections to classical molecular dynamics studies. <i>Journal of Chemical Physics</i> , 2016, 144, 124512.	1.2	20
20	Direct phase coexistence molecular dynamics study of the phase equilibria of the ternary methane-carbon dioxide-water hydrate system. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 23538-23548.	1.3	39
21	Storage of Methane in Clathrate Hydrates: Monte Carlo Simulations of sI Hydrates and Comparison with Experimental Measurements. <i>Journal of Chemical & Engineering Data</i> , 2016, 61, 2886-2896.	1.0	26
22	Molecular dynamics simulations of pure methane and carbon dioxide hydrates: lattice constants and derivative properties. <i>Molecular Physics</i> , 2016, 114, 2672-2687.	0.8	24
23	Development of a novel experimental apparatus for hydrate equilibrium measurements. <i>Fluid Phase Equilibria</i> , 2016, 424, 152-161.	1.4	10
24	Microscale characterisation of stochastically reconstructed carbon fiber-based Gas Diffusion Layers; effects of anisotropy and resin content. <i>Journal of Power Sources</i> , 2016, 320, 153-167.	4.0	30
25	Comparing hydrogen sorption in different Pd-doped pristine and surface-modified nanoporous carbons. <i>Carbon</i> , 2016, 98, 1-14.	5.4	11
26	The role of intermolecular interactions in the prediction of the phase equilibria of carbon dioxide hydrates. <i>Journal of Chemical Physics</i> , 2015, 143, 094506.	1.2	58
27	Prediction of the phase equilibria of methane hydrates using the direct phase coexistence methodology. <i>Journal of Chemical Physics</i> , 2015, 142, 044501.	1.2	111
28	Gas Solubility in Aqueous Solutions Under Two-Phase (H ₂ O-Lw) Hydrate Equilibrium Conditions. , 2015, , 205-212.		0
29	A generic physical model for a thermally integrated high-temperature PEM fuel cell and sodium alanate tank system. <i>International Journal of Hydrogen Energy</i> , 2015, 40, 14551-14561.	3.8	12
30	A complete transport validated model on a zeolite membrane for carbon dioxide permeance and capture. <i>Applied Thermal Engineering</i> , 2015, 74, 36-46.	3.0	14
31	Influence of combining rules on the cavity occupancy of clathrate hydrates using van der Waals-Platteeuw-theory-based modelling. <i>Chemical Engineering Research and Design</i> , 2014, 92, 2992-3007.	2.7	12
32	High-temperature activated AB ₂ nanopowders for metal hydride hydrogen compression. <i>International Journal of Energy Research</i> , 2014, 38, 477-486.	2.2	19
33	Influence of combining rules on the cavity occupancy of clathrate hydrates by Monte Carlo simulations. <i>Molecular Physics</i> , 2014, 112, 2258-2274.	0.8	32
34	Methane solubility in aqueous solutions under two-phase (H ₂ O-Lw) hydrate equilibrium conditions. <i>Fluid Phase Equilibria</i> , 2014, 371, 106-120.	1.4	37
35	The required level of isosteric heat for the adsorptive/storage delivery of H ₂ in the UiO series of MOFs. <i>RSC Advances</i> , 2014, 4, 44848-44851.	1.7	4
36	Thermal coupling potential of Solid Oxide Fuel Cells with metal hydride tanks: Thermodynamic and design considerations towards integrated systems. <i>Journal of Power Sources</i> , 2014, 269, 440-450.	4.0	22

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37	Newtonian and Power-Law fluid flow in a T-junction of rectangular ducts. Theoretical and Computational Fluid Dynamics, 2014, 28, 233-256.	0.9	18
38	Investigation of ZrFe ₂ -type materials for metal hydride hydrogen compressor systems by substituting Fe with Cr or V. International Journal of Hydrogen Energy, 2014, 39, 21380-21385.	3.8	31
39	Hydrogen sorption properties of Pd-doped carbon molecular sieves. International Journal of Hydrogen Energy, 2014, 39, 9830-9836.	3.8	16
40	A hydrogen sorption study on a Pd-doped CMK-3 type ordered mesoporous carbon. Adsorption, 2013, 19, 803-811.	1.4	9
41	Polymer-stable magnesium nanocomposites prepared by laser ablation for efficient hydrogen storage. International Journal of Hydrogen Energy, 2013, 38, 11530-11535.	3.8	79
42	Techno-economic analysis of RES & hydrogen technologies integration in remote island power system. International Journal of Hydrogen Energy, 2013, 38, 11646-11654.	3.8	22
43	The effect of compositional changes on the structural and hydrogen storage properties of (La ^{1-x} Ce ^x)Ni ₅ type intermetallics towards compounds suitable for metal hydride hydrogen compression. Journal of Alloys and Compounds, 2013, 580, S268-S270.	2.8	52
44	Synthesis and Characterization of TiFe _{0.7} Mn _{0.3} V _x (<i>x</i> = 0.05, and 0.1) and Ti _{1-x} Ta _x Fe _{0.7} Mn _{0.3} (<i>x</i> = 0.2, and) Tj ETQ 0 0 0 BT / Overlo		
45	Structural Microchemistry, and Hydrogenation Properties of TiMn _{0.4} Fe _{0.2} V _{0.4} , TiMn _{0.1} Fe _{0.2} V _{0.7} and Ti _{0.4} Zr _{0.6} Mn _{0.4} Fe _{0.2} V _{0.4} Metal Hydrides. Journal of Nanoscience and Nanotechnology, 2012, 12, 1688-1696.	0.9	3
46	Synthesis and characterisation of a mesoporous carbon/calcium borohydride nanocomposite for hydrogen storage. International Journal of Hydrogen Energy, 2012, 37, 16631-16635.	3.8	17
47	On the limitation of the van der Waals-Platteeuw-based thermodynamic models for hydrates with multiple occupancy of cavities. Molecular Physics, 2012, 110, 1213-1221.	0.8	24
48	Synthesis and characterisation of nanoporous carbon-metal composites for hydrogen storage. Microporous and Mesoporous Materials, 2012, 154, 74-81.	2.2	17
49	Enhanced hydrogen storage by spillover on metal-doped carbon foam: an experimental and computational study. Nanoscale, 2011, 3, 933.	2.8	65
50	Experimental and Computational Investigation of the sll Binary He ¹³ THF Hydrate. Journal of Physical Chemistry B, 2011, 115, 1411-1415.	1.2	29
51	Scale prediction in liquid flow through porous media: A geochemical model for the simulation of CaCO ₃ deposition at the near-well region. Journal of Geochemical Exploration, 2011, 108, 115-125.	1.5	18
52	Hydrogenation properties of the TiB _x structures. International Journal of Hydrogen Energy, 2011, 36, 12268-12278.	3.8	5
53	A Lattice Boltzmann Method for Non Ideal Gases Based on the Gradient Theory of Interfaces. Computer Aided Chemical Engineering, 2011, 29, 1598-1602.	0.3	0
54	Determination of the spatial distribution of multiple fluid phases in porous media by ultra-small-angle neutron scattering. Applied Surface Science, 2010, 256, 5329-5333.	3.1	2

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55	Application of the Lattice-Boltzmann method to the modeling of population blob dynamics in 2D porous domains. <i>Computers and Mathematics With Applications</i> , 2010, 59, 2315-2325.	1.4	6
56	Graphene Fluoride: A Stable Stoichiometric Graphene Derivative and its Chemical Conversion to Graphene. <i>Small</i> , 2010, 6, 2885-2891.	5.2	386
57	Fractal Characteristics and Scaling of the Drying Front in Porous Media: A Pore Network Study. <i>Drying Technology</i> , 2010, 28, 981-990.	1.7	29
58	Unexpected Behavior of Helium as Guest Gas in sII Binary Hydrates. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1014-1017.	2.1	30
59	Monte Carlo study of sI hydrogen hydrates. <i>Molecular Simulation</i> , 2010, 36, 736-744.	0.9	14
60	Structural and Electronic Properties of the Hydrogenated ZrCr ₂ Laves Phases. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4221-4227.	1.5	17
61	Liquid-Phase Exfoliation of Graphite Towards Solubilized Graphenes. <i>Small</i> , 2009, 5, 1841-1845.	5.2	508
62	Modeling and optimization of multi-tubular metal hydride beds for efficient hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2009, 34, 9128-9140.	3.8	54
63	Aqueous-phase exfoliation of graphite in the presence of polyvinylpyrrolidone for the production of water-soluble graphenes. <i>Solid State Communications</i> , 2009, 149, 2172-2176.	0.9	255
64	A hybrid process-based and stochastic reconstruction method of porous media. <i>Microporous and Mesoporous Materials</i> , 2008, 110, 92-99.	2.2	56
65	Monte Carlo study of sII and sH argon hydrates with multiple occupancy of cages. <i>Molecular Simulation</i> , 2008, 34, 1311-1320.	0.9	27
66	Why Li Doping in MOFs Enhances H ₂ Storage Capacity? A Multi-scale Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2008, 112, 7290-7294.	1.5	145
67	Hydrogen Storage in sH Hydrates: A Monte Carlo Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14206-14211.	1.2	47
68	Evaluation of the Hydrogen-Storage Capacity of Pure H ₂ and Binary H ₂ -THF Hydrates with Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10294-10302.	1.5	81
69	Coupling between external and internal mass transfer during drying of a porous medium. <i>Water Resources Research</i> , 2007, 43, .	1.7	80
70	Characterization of nanoporous carbons by combining CO ₂ and H ₂ sorption data with the Monte Carlo simulations. <i>Applied Surface Science</i> , 2007, 253, 5715-5720.	3.1	23
71	Atomistic simulation of sorption in model pores with reduced spatial periodicity. <i>Applied Surface Science</i> , 2007, 253, 5606-5609.	3.1	3
72	A lattice Boltzmann study of viscous coupling effects in immiscible two-phase flow in porous media. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2007, 300, 35-49.	2.3	126

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73	Synthesis, characterization and gas sorption properties of a molecularly-derived graphite oxide-like foam. <i>Carbon</i> , 2007, 45, 852-857.	5.4	60
74	Preparation and characterisation of gas selective microporous carbon membranes. <i>Microporous and Mesoporous Materials</i> , 2007, 99, 181-189.	2.2	34
75	Experimental investigation of asphaltene deposition mechanism during oil flow in core samples. <i>Journal of Petroleum Science and Engineering</i> , 2007, 57, 281-293.	2.1	88
76	A Lattice Boltzmann study of non-newtonian flow in digitally reconstructed porous domains. <i>Transport in Porous Media</i> , 2007, 70, 279-292.	1.2	27
77	Multi-scale modelling and optimization of hydrogen storage systems using advanced solid materials. <i>Computer Aided Chemical Engineering</i> , 2006, 21, 185-190.	0.3	0
78	Study of Calcium Carbonate Precipitation in the Near-Well Region Using ⁴⁷ Ca as Tracer. <i>SPE Production and Operations</i> , 2006, 21, 33-39.	0.4	3
79	Dynamic modelling and optimization of hydrogen storage in metal hydride beds. <i>Energy</i> , 2006, 31, 2428-2446.	4.5	56
80	An integrated radiotracer approach for the laboratory evaluation of scale inhibitors performance in geological environments. <i>Chemical Engineering Science</i> , 2006, 61, 7057-7067.	1.9	16
81	On the optimization of hydrogen storage in metal hydride beds. <i>International Journal of Hydrogen Energy</i> , 2006, 31, 737-751.	3.8	78
82	Pore-network study of the characteristic periods in the drying of porous materials. <i>Journal of Colloid and Interface Science</i> , 2006, 297, 738-748.	5.0	145
83	Multiphase mass transport with partitioning and inter-phase transport in porous media. <i>Chemical Engineering Science</i> , 2006, 61, 4650-4661.	1.9	30
84	Multiscale modeling and optimization of H ₂ storage using nanoporous adsorbents. <i>AIChE Journal</i> , 2006, 52, 2964-2977.	1.8	7
85	An improved predictive correlation for the induction time of CaCO ₃ scale formation during flow in porous media. <i>Journal of Colloid and Interface Science</i> , 2005, 286, 7-13.	5.0	31
86	Low to moderate Peclet mass transport in assemblages of spherical particles for a realistic adsorption–reaction–desorption mechanism. <i>Powder Technology</i> , 2005, 159, 173-179.	2.1	7
87	Combination of small angle neutron scattering data and mesoscopic simulation techniques as a tool for the structural characterization and prediction of properties of bi-phasic media. <i>Chemical Physics</i> , 2005, 317, 298-311.	0.9	11
88	Use of natural geochemical tracers to improve reservoir simulation models. <i>Journal of Petroleum Science and Engineering</i> , 2005, 48, 241-253.	2.1	27
89	On the identification of representative samples from large data sets, with application to synoptic climatology. <i>Theoretical and Applied Climatology</i> , 2005, 82, 177-182.	1.3	8
90	Digitally Reconstructed Porous Media: Transport and Sorption Properties. <i>Transport in Porous Media</i> , 2005, 58, 43-62.	1.2	38

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91	Effect of liquid films on the drying of porous media. <i>AIChE Journal</i> , 2004, 50, 2721-2737.	1.8	171
92	Structural alterations of fully hydrated human stratum corneum. <i>Physica B: Condensed Matter</i> , 2004, 350, E603-E606.	1.3	29
93	Transport of organic components from immobile and bypassed oil in porous media. <i>AIChE Journal</i> , 2003, 49, 1085-1094.	1.8	4
94	Low Peclet mass transport in assemblages of spherical particles for two different adsorption mechanisms. <i>Journal of Colloid and Interface Science</i> , 2003, 264, 20-29.	5.0	22
95	Simulated Annealing as a Method for the Determination of the Spatial Distribution of a Condensable Adsorbate in Mesoporous Materials. <i>Langmuir</i> , 2003, 19, 3333-3337.	1.6	9
96	Origin of Hysteresis of Gas Adsorption in Disordered Porous Media: A Lattice Gas Model versus Percolation Theory. <i>Langmuir</i> , 2003, 19, 3338-3344.	1.6	21
97	The effect of Peclet on the Sherwood number in high porosity granular media. <i>Studies in Surface Science and Catalysis</i> , 2002, 144, 753-760.	1.5	4
98	A Monte Carlo study on the structure of carbon dioxide adsorbed in microporous carbons. <i>Studies in Surface Science and Catalysis</i> , 2002, 144, 545-552.	1.5	8
99	A neutron-diffraction study of the effect of hydration on stratum corneum structure. <i>Applied Physics A: Materials Science and Processing</i> , 2002, 74, s1245-s1247.	1.1	15
100	Diffusion and Flow in Porous Domains Constructed Using Process-Based and Stochastic Techniques. <i>Journal of Porous Materials</i> , 2002, 9, 141-154.	1.3	29
101	Simulation Study of Sorption of CO ₂ and N ₂ with Application to the Characterization of Carbon Adsorbents. <i>Molecular Simulation</i> , 2001, 27, 441-456.	0.9	17
102	A 2-D pore-network model of the drying of single-component liquids in porous media. <i>Advances in Water Resources</i> , 2001, 24, 439-460.	1.7	133
103	Phase change in porous media. <i>Current Opinion in Colloid and Interface Science</i> , 2001, 6, 208-216.	3.4	62
104	Numerical and experimental investigation of the diffusional release of a dispersed solute from polymeric multilaminate matrices. <i>Journal of Controlled Release</i> , 2001, 70, 309-319.	4.8	30
105	Structural Characterisation and Applications of Ceramic Membranes for Gas Separations. <i>Studies in Surface Science and Catalysis</i> , 2000, 128, 429-438.	1.5	1
106	Adsorption-Desorption Flow of Condensable Vapors through Mesoporous Media: Network Modeling and Percolation Theory. <i>Journal of Colloid and Interface Science</i> , 2000, 223, 89-101.	5.0	6
107	The Structure of Adsorbed CO ₂ in Slitlike Micropores at Low and High Temperature and the Resulting Micropore Size Distribution Based on GCMC Simulations. <i>Journal of Colloid and Interface Science</i> , 2000, 224, 272-290.	5.0	43
108	Structural and Transport Properties of Alumina Porous Membranes from Process-Based and Statistical Reconstruction Techniques. <i>Journal of Colloid and Interface Science</i> , 2000, 231, 158-167.	5.0	36

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109	Pore geometry and transport properties in North Sea chalk. Journal of Petroleum Science and Engineering, 2000, 25, 107-134.	2.1	43
110	A study on structural and diffusion properties of porcine stratum corneum based on very small angle neutron scattering data. Pharmaceutical Research, 2000, 17, 1085-1091.	1.7	29
111	Combination of small angle scattering and three-dimensional stochastic reconstruction for the study of adsorption-desorption processes in Vycor porous glass. Journal of Chemical Physics, 2000, 112, 9881-9887.	1.2	37
112	Evaporation of a Stagnant Liquid. Industrial & Engineering Chemistry Research, 2000, 39, 1505-1513.	1.8	10
113	Ceramic membranes - characterization and applications. Studies in Surface Science and Catalysis, 1999, 120, 687-713.	1.5	3
114	Simulation of self-diffusion of point-like and finite-size tracers in stochastically reconstructed Vycor porous glasses. Journal of Chemical Physics, 1999, 111, 2735-2743.	1.2	42
115	Scaling theory of drying in porous media. Physical Review E, 1999, 59, 4353-4365.	0.8	101
116	AERODYNAMICALLY GENERATED ACOUSTIC RESONANCE IN A PIPE WITH ANNULAR FLOW RESTRICTORS. Journal of Fluids and Structures, 1999, 13, 755-778.	1.5	23
117	PEEL ADHESION PROPERTIES OF AIR-DRIED PHARMACEUTICAL PRESSURE SENSITIVE ADHESIVE. Drying Technology, 1999, 17, 2093-2106.	1.7	0
118	DRYING KINETICS OF A MULTICOMPONENT MIXTURE OF ORGANIC SOLVENTS. Drying Technology, 1999, 17, 2107-2122.	1.7	4
119	Adsorption-desorption gas relative permeability through mesoporous media-network modelling and percolation theory. Chemical Engineering Science, 1998, 53, 2353-2364.	1.9	29
120	A two-phase model for controlled drug release from biphasic polymer hydrogels. Journal of Controlled Release, 1998, 51, 313-325.	4.8	19
121	A novel experimental technique for the measurement of the single-phase gas relative permeability of porous solids. Measurement Science and Technology, 1997, 8, 168-173.	1.4	24
122	Determination of Micropore Size Distribution from Grand Canonical Monte Carlo Simulations and Experimental CO2 Isotherm Data. Langmuir, 1997, 13, 2795-2802.	1.6	108
123	High pressure gas permeability of microporous carbon membranes. Microporous Materials, 1997, 8, 171-176.	1.6	77
124	Application of effective medium approximation for the determination of the permeability of condensable vapours through mesoporous media. Chemical Engineering Science, 1997, 52, 2837-2844.	1.9	22
125	Novel design for high pressure, integral, differential, absolute, and relative multicomponent permeability measurements. Review of Scientific Instruments, 1996, 67, 2545-2548.	0.6	25
126	Water adsorption and small angle X-ray scattering studies on the effect of coal thermal treatment. Carbon, 1996, 34, 775-781.	5.4	14

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127	A network model for the permeability of condensable vapours through mesoporous media. Journal of Membrane Science, 1996, 114, 215-225.	4.1	32