Said Hamad

List of Publications by Year
in descending order

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Version: 2024-02-01

75 papers	3,256 citations	109321 35 h-index	149698 56 g-index
78 all docs	78 docs citations	78 times ranked	4608 citing authors

#	Article	IF	Citations
1	Thermostructural Characterization of Silicon Carbide Nanocomposite Materials via Molecular Dynamics Simulations. Advanced Composite Materials, 2022, 31, 485-504.	1.9	0
2	Unravelling the key factors in the chlorine-promoted epoxidation of ethylene over a silverâ€“copper oxide nanocatalyst. Nanoscale, 2022, 14, 7332-7340.	5.6	3
3	Engineering the electronic and optical properties of 2D porphyrin-paddlewheel metal-organic frameworks. JPhys Energy, 2021, 3, 034005.	5.3	7
4	Bandgap Engineering in the Configurational Space of Solid Solutions via Machine Learning: (Mg,Zn)O Case Study. Journal of Physical Chemistry Letters, 2021, 12, 5163-5168.	4.6	8
5	Molecular Dynamics Analysis of Charge Transport in Ionicâ€Liquid Electrolytes Containing Added Salt with Mono, Di, and Trivalent Metal Cations. ChemPhysChem, 2018, 19, 1665-1673.	2.1	23
6	The Siâ€“Ge substitutional series in the chiral STW zeolite structure type. Journal of Materials Chemistry A, 2018, 6, 15110-15122.	10.3	33
7	Role of Ionic Liquid [EMIM]⁺[SCN]^{â^'} in the Adsorption and Diffusion of Gases in Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2018, 10, 29694-29704.	8.0	38
8	Fitting electron density as a physically sound basis for the development of interatomic potentials of complex alloys. Physical Chemistry Chemical Physics, 2018, 20, 18647-18656.	2.8	2
9	Electrochemical Reduction of Oxygen in Aprotic Ionic Liquids Containing Metal Cations: A Case Study on the Naâ€“O₂ system. ChemSusChem, 2017, 10, 1616-1623.	6.8	30
10	Importance of Blocking Inaccessible Voids on Modeling Zeolite Adsorption: Revisited. Journal of Physical Chemistry C, 2017, 121, 4462-4470.	3.1	17
11	Selective sulfur dioxide adsorption on crystal defect sites on an isoreticular metal organic framework series. Nature Communications, 2017, 8, 14457.	12.8	133
12	Porphyrin-based metal-organic frameworks for solar fuel synthesis photocatalysis: band gap tuning via iron substitutions. Journal of Materials Chemistry A, 2017, 5, 11894-11904.	10.3	84
13	On the ionophoric selectivity of nonactin and related macrotetrolide derivatives. Physical Chemistry Chemical Physics, 2017, 19, 1288-1297.	2.8	6
14	Tuning the separation properties of zeolitic imidazolate framework coreâ€“shell structures via post-synthetic modification. Journal of Materials Chemistry A, 2017, 5, 25601-25608.	10.3	56
15	Critical Role of Dynamic Flexibility in Geâ€Containing Zeolites: Impact on Diffusion. Chemistry - A European Journal, 2016, 22, 10036-10043.	3.3	22
16	Frontispiz: Modelling a Linker Mix-and-Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, .	2.0	0
17	Frontispiece: Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, .	13.8	1
18	Ab initio molecular dynamics investigation of proton delocalization in crown ether complexes with H3O+ and NH4 +. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 85, 83-92.	1.6	6

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19	High Capacity Naâ€“O₂ Batteries: Key Parameters for Solution-Mediated Discharge. Journal of Physical Chemistry C, 2016, 120, 20068-20076.	3.1	96
20	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie - International Edition, 2016, 55, 16012-16016.	13.8	61
21	Modelling a Linker Mixâ€andâ€Match Approach for Controlling the Optical Excitation Gaps and Band Alignment of Zeolitic Imidazolate Frameworks. Angewandte Chemie, 2016, 128, 16246-16250.	2.0	12
22	Controlling Thermal Expansion: A Metalâ€“Organic Frameworks Route. Chemistry of Materials, 2016, 28, 8296-8304.	6.7	42
23	Liquid self-diffusion of H₂O and DMF molecules in Co-MOF-74: molecular dynamics simulations and dielectric spectroscopy studies. Physical Chemistry Chemical Physics, 2016, 18, 19605-19612.	2.8	21
24	Quantum and Classical Molecular Dynamics of Ionic Liquid Electrolytes for Na/Liâ€based Batteries: Molecular Origins of the Conductivity Behavior. ChemPhysChem, 2016, 17, 2473-2481.	2.1	29
25	Comparing gas separation performance between all known zeolites and their zeolitic imidazolate framework counterparts. Dalton Transactions, 2016, 45, 216-225.	3.3	26
26	Binding Selectivity of Macrocycle Ionophores in Ionic Liquids versus Aqueous Solution and Solventâ€free Conditions. ChemPhysChem, 2015, 16, 3672-3680.	2.1	5
27	Ultraviolet Pretreatment of Titanium Dioxide and Tin-Doped Indium Oxide Surfaces as a Promoter of the Adsorption of Organic Molecules in Dry Deposition Processes: Light Patterning of Organic Nanowires. Langmuir, 2015, 31, 8294-8302.	3.5	5
28	Thermostructural behaviour of Niâ€“Cr materials: modelling of bulk and nanoparticle systems. Physical Chemistry Chemical Physics, 2015, 17, 15912-15920.	2.8	13
29	Understanding Nanopore Window Distortions in the Reversible Molecular Valve Zeolite RHO. Chemistry of Materials, 2015, 27, 5657-5667.	6.7	42
30	Electronic structure of porphyrin-based metalâ€“organic frameworks and their suitability for solar fuel production photocatalysis. Journal of Materials Chemistry A, 2015, 3, 23458-23465.	10.3	59
31	Atomic charges for modeling metalâ€“organic frameworks: Why and how. Journal of Solid State Chemistry, 2015, 223, 144-151.	2.9	47
32	Ion Transport in Electrolytes for Dye-Sensitized Solar Cells: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry C, 2014, 118, 28448-28455.	3.1	14
33	Molecular simulation of gas adsorption and diffusion in a breathing MOF using a rigid force field. Physical Chemistry Chemical Physics, 2014, 16, 16060-16066.	2.8	31
34	Adsorption of hydrogen sulphide on Metal-Organic Frameworks. RSC Advances, 2013, 3, 14737.	3.6	49
35	Toward a Transferable Set of Charges to Model Zeolitic Imidazolate Frameworks: Combined Experimentalâ€“Theoretical Research. Journal of Physical Chemistry C, 2013, 117, 466-471.	3.1	24
36	Understanding Adsorption of Highly Polar Vapors on Mesoporous MIL-100(Cr) and MIL-101(Cr): Experiments and Molecular Simulations. Journal of Physical Chemistry C, 2013, 117, 7613-7622.	3.1	79

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37	Multipodal coordination of a tetracarboxylic crown ether with NH 4+: A vibrational spectroscopy and computational study. Journal of Chemical Physics, 2012, 136, 114301.	3.0	8
38	Tweezerâ€like Complexes of Crown Ethers with Divalent Metals: Probing Cationâ€Sizeâ€Dependent Conformations by Vibrational Spectroscopy in the Gas Phase. ChemPlusChem, 2012, 77, 118-123.	2.8	11
39	Effect of air humidity on the removal of carbon tetrachloride from air using Cuâ€“BTC metalâ€“organic framework. Physical Chemistry Chemical Physics, 2011, 13, 11165.	2.8	40
40	On the performance of Cu-BTC metal organic framework for carbon tetrachloride gas removal. Chemical Communications, 2011, 47, 508-510.	4.1	32
41	Are glycine cyclic dimers stable in aqueous solution?. CrystEngComm, 2011, 13, 4391.	2.6	18
42	Crown Ether Complexes with H₃O⁺ and NH₄⁺: Proton Localization and Proton Bridge Formation. Journal of Physical Chemistry A, 2011, 115, 7275-7282.	2.5	55
43	Phase separation and surface segregation in ceriaâ€“zirconia solid solutions. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 1925-1938.	2.1	45
44	Emergence of Symmetry and Chirality in Crown Ether Complexes with Alkali Metal Cations. Journal of Physical Chemistry A, 2010, 114, 7048-7054.	2.5	64
45	Modelling nano-clusters and nucleation. Physical Chemistry Chemical Physics, 2010, 12, 786-811.	2.8	174
46	Performance of Chiral Zeolites for Enantiomeric Separation Revealed by Molecular Simulation. Journal of Physical Chemistry C, 2010, 114, 22207-22213.	3.1	34
47	Band Gap Narrowing versus Formation of Electronic States in the Gap in Nâ¯TiO₂ Thin Films. Journal of Physical Chemistry C, 2010, 114, 22546-22557.	3.1	34
48	Exploration of multiple energy landscapes for zirconia nanoclusters. Physical Chemistry Chemical Physics, 2010, 12, 8454.	2.8	26
49	Gasâ€“phase complexes of cyclic and linear polyethers with alkali cations. Physical Chemistry Chemical Physics, 2010, 12, 13752.	2.8	31
50	Incorporation and Thermal Evolution of Rhodamine 6G Dye Molecules Adsorbed in Porous Columnar Optical SiO2 Thin Films. Langmuir, 2009, 25, 9140-9148.	3.5	30
51	Experimental and computational studies of ZnS nanostructures. Molecular Simulation, 2009, 35, 1015-1032.	2.0	54
52	Molecular Insights into the Self-Aggregation of Aromatic Molecules in the Synthesis of Nanoporous Aluminophosphates: A Multilevel Approach. Journal of the American Chemical Society, 2009, 131, 16509-16524.	13.7	35
53	Molecular dynamics simulation of the effect of pH on the adsorption of rhodamine laser dyes on TiO₂hydroxylated surfaces. Molecular Simulation, 2009, 35, 1140-1151.	2.0	15
54	Changing the physical and chemical properties of titanium oxynitrides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiN</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:m changing the composition. Physical Review B, 2009, 80, .	3.2	48

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55	Clustering of Glycine Molecules in Aqueous Solution Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 7280-7288.	2.6	79
56	Low reactivity of non-bridging oxygen defects on stoichiometric silica surfaces. Chemical Communications, 2008, , 4156.	4.1	20
57	Modelling nucleation and nano-particle structures. Molecular Physics, 2007, 105, 177-187.	1.7	9
58	A multi-technique approach for probing the evolution of structural properties during crystallization of organic materials from solution. Faraday Discussions, 2007, 136, 71.	3.2	58
59	Symmetry-adapted configurational modelling of fractional site occupancy in solids. Journal of Physics Condensed Matter, 2007, 19, 256201.	1.8	182
60	Kinetic Insights into the Role of the Solvent in the Polymorphism of 5-Fluorouracil from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 3323-3329.	2.6	107
61	Applications Of Dl_poly And Dl_multi To Organic Molecular Crystals. Molecular Simulation, 2006, 32, 985-997.	2.0	27
62	Properties of small TiO2, ZrO2and HfO2nanoparticles. Journal of Materials Chemistry, 2006, 16, 1927-1933.	6.7	69
63	Computational study of the relative stabilities of ZnS clusters, for sizes between 1 and 4nm. Journal of Crystal Growth, 2006, 294, 2-8.	1.5	51
64	Electronic excitation energies of ZniSinanoparticles. Nanotechnology, 2006, 17, 4100-4105.	2.6	16
65	Structure and Stability of Small TiO2Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 15741-15748.	2.6	212
66	Structure and Properties of ZnS Nanoclusters. ChemInform, 2005, 36, no.	0.0	0
67	Simulation of the Embryonic Stage of ZnS Formation from Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 2580-2590.	13.7	38
68	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	2.6	102
69	Theoretical Study of the Adsorption of Water on a Model Soot Surface:Â I. Quantum Chemical Calculations. Journal of Physical Chemistry B, 2004, 108, 5405-5409.	2.6	43
70	Theoretical Study of the Adsorption of Water on a Model Soot Surface:Â II. Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 5410-5415.	2.6	44
71	ZnS bubble clusters with onion-like structures. Chemical Communications, 2004, , 864-865.	4.1	51
72	Computational Evidence of Bubble ZnS Clusters. Journal of Physical Chemistry B, 2003, 107, 10337-10340.	2.6	82

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73	A Computational Study of the Hydration of the OH Radical. Journal of Physical Chemistry A, 2002, 106, 9104-9113.	2.5	59
74	Surface Structures and Crystal Morphology of ZnS:â€‰ Computational Study. Journal of Physical Chemistry B, 2002, 106, 11002-11008.	2.6	116
75	Calculation of the Free Energy of Proton Transfer from an Aqueous Phase to Liquid Acetonitrile. Journal of Physical Chemistry B, 2001, 105, 9872-9878.	2.6	13