George E Froudakis

List of Publications by Year
in descending order

130 papers	7,968 citations	61984 43 h-index	49909 87 g-index
131 all docs	131 docs citations	131 times ranked	8802 citing authors

#	Article	IF	Citations
1	Introducing artificial MOFs for improved machine learning predictions: Identification of top-performing materials for methane storage. Journal of Chemical Physics, 2022, 156, 054103.	3.0	9
2	Linker Functionalization Strategy for Water Adsorption in Metalâ€“Organic Frameworks. Molecules, 2022, 27, 2614.	3.8	7
3	Surface Modification Strategy for Enhanced NO2 Capture in Metalâ€“Organic Frameworks. Molecules, 2022, 27, 3448.	3.8	5
4	Enhancing of CO Uptake in Metal-Organic Frameworks by Linker Functionalization: A Multi-Scale Theoretical Study. Chemistry, 2022, 4, 603-614.	2.2	4
5	SiPM-matrix readout of two-phase argon detectors using electroluminescence in the visible and near infrared range. European Physical Journal C, 2021, 81, 1.	3.9	18
6	Continuous Breathing Rare-Earth MOFs Based on Hexanuclear Clusters with Gas Trapping Properties. Journal of the American Chemical Society, 2021, 143, 10250-10260.	13.7	30
7	A combination of multi-scale calculations with machine learning for investigating hydrogen storage in metal organic frameworks. International Journal of Hydrogen Energy, 2021, 46, 27612-27621.	7.1	25
8	Expanding the NUIG MOF family: synthesis and characterization of new MOFs for selective CO₂ adsorption, metal ion removal from aqueous systems, and drug delivery applications. Dalton Transactions, 2021, 50, 6997-7006.	3.3	11
9	Two-Fold Homointerpenetrated Metalâ€“Organic Framework with the Potential for Anticancer Drug Loading Using Computational Simulations. Crystal Growth and Design, 2021, 21, 6402-6410.	3.0	7
10	Water-stable 2-D Zr MOFs with exceptional UO₂²⁺ sorption capability. Journal of Materials Chemistry A, 2020, 8, 1849-1857.	10.3	29
11	Materials for hydrogen-based energy storage â€“ past, recent progress and future outlook. Journal of Alloys and Compounds, 2020, 827, 153548.	5.5	518
12	Porous carbon nanotube networks and pillared graphene materials exhibiting high SF6 adsorption uptake and separation selectivity of SF6/N2 fluid mixtures: A comparative molecular simulation study. Microporous and Mesoporous Materials, 2020, 307, 110464.	4.4	16
13	Fast Screening of Large Databases for Top Performing Nanomaterials Using a Self-Consistent, Machine Learning Based Approach. Journal of Physical Chemistry C, 2020, 124, 19639-19648.	3.1	22
14	Confinement Effects on the Properties of Polar Hydrogen-Bonded Fluids: A Showcase on Methanol Adsorbed in Three-Dimensional Pillared Graphene and Carbon Nanotube Networks. Journal of Physical Chemistry C, 2020, 124, 22959-22971.	3.1	4
15	A biocompatible ZnNa2-based metalâ€“organic framework with high ibuprofen, nitric oxide and metal uptake capacity. Materials Advances, 2020, 1, 2248-2260.	5.4	8
16	A Generic Machine Learning Algorithm for the Prediction of Gas Adsorption in Nanoporous Materials. Journal of Physical Chemistry C, 2020, 124, 7117-7126.	3.1	51
17	An Automated Machine Learning architecture for the accelerated prediction of Metal-Organic Frameworks performance in energy and environmental applications. Microporous and Mesoporous Materials, 2020, 300, 110160.	4.4	40
18	A Universal Machine Learning Algorithm for Large-Scale Screening of Materials. Journal of the American Chemical Society, 2020, 142, 3814-3822.	13.7	98

#	Article	IF	Citations
19	Organically interconnected graphene flakes: A flexible 3-D material with tunable electronic bandgap. Scientific Reports, 2019, 9, 13676.	3.3	5
20	A Robust Machine Learning Algorithm for the Prediction of Methane Adsorption in Nanoporous Materials. Journal of Physical Chemistry A, 2019, 123, 6080-6087.	2.5	61
21	Review of computer simulations on anti-cancer drug delivery in MOFs. Inorganic Chemistry Frontiers, 2018, 5, 1255-1272.	6.0	79
22	DarkSide-20k: A 20 tonne two-phase LAr TPC for direct dark matter detection at LNGS. European Physical Journal Plus, 2018, 133, 1.	2.6	247
23	Directed assembly of a high surface area 2D metalâ€“organic framework displaying the augmented â€œkagomÃ© dualâ€•(kgd-a) layered topology with high H₂and CO₂uptake. Inorganic Chemistry Frontiers, 2017, 4, 825-832.	6.0	8
24	Multiscale simulations reveal IRMOF-74-III as a potent drug carrier for gemcitabine delivery. Journal of Materials Chemistry B, 2017, 5, 3277-3282.	5.8	49
25	Antimony speciation in spirits stored in PET bottles: identification of a novel antimony complex. Journal of Analytical Atomic Spectrometry, 2017, 32, 1109-1118.	3.0	7
26	Chemically intuited, large-scale screening of MOFs by machine learning techniques. Npj Computational Materials, 2017, 3, .	8.7	107
27	OH-functionalization strategy in Metal-Organic Frameworks for drug delivery. Chemical Physics Letters, 2017, 685, 114-118.	2.6	20
28	Reticular Chemistry and the Discovery of a New Family of Rare Earth (4, 8)-Connected Metal-Organic Frameworks with csq Topology Based on RE₄(Î¼₃-O)₂(COO)₈ Clusters. ACS Applied Materials & Interfaces, 2017, 9, 44560-44566.	8.0	25
29	Cryogenic Characterization of FBK RGB-HD SiPMs. Journal of Instrumentation, 2017, 12, P09030-P09030.	1.2	16
30	Outlook and challenges for hydrogen storage in nanoporous materials. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	2.3	129
31	Highly selective separation and adsorption-induced phase transition of SF 6 -N 2 fluid mixtures in three-dimensional carbon nanotube networks. Journal of Supercritical Fluids, 2016, 113, 89-95.	3.2	8
32	Tuning the interaction strength and the adsorption of CO2 in metal organic frameworks by functionalization of the organic linkers. Microporous and Mesoporous Materials, 2016, 227, 144-151.	4.4	28
33	Reticular Synthesis of HKUST-like tbo-MOFs with Enhanced CH₄ Storage. Journal of the American Chemical Society, 2016, 138, 1568-1574.	13.7	193
34	Enhancement of CO₂ Adsorption in Magnesium Alkoxide IRMOF-10. Journal of Physical Chemistry C, 2015, 119, 22001-22007.	3.1	9
35	Alternative use of cross-linked polyallylamine (known as Sevelamer pharmaceutical compound) as biosorbent. Journal of Colloid and Interface Science, 2015, 442, 49-59.	9.4	11
36	Direct observation of spin-injection in tyrosinate-functionalized single-wall carbon nanotubes. Carbon, 2014, 67, 424-433.	10.3	7

#	Article	IF	Citations
37	Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 9825-9829.	7.1	30
38	Ab Initio Study of the Adsorption of CO₂ on Functionalized Benzenes. ChemPhysChem, 2014, 15, 905-911.	2.1	15
39	Drastic Enhancement of the CO₂ Adsorption Properties in Sulfone-Functionalized Zr- and Hf-UiO-67 MOFs with Hierarchical Mesopores. Inorganic Chemistry, 2014, 53, 679-681.	4.0	87
40	Separation of CO₂â€“N₂mixtures in 3D carbon-based porous nanotube networks: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2014, 16, 876-879.	2.8	14
41	A â€œturn-onâ€â€“turning-to-ratiometric sensor for zinc(<scp>ii</scp>) ions in aqueous media. RSC Advances, 2014, 4, 693-696.	3.6	10
42	Hydrogen Storage with Spectroscopic Identification of Chemisorption Sites in Cu-TDPAT via Spillover from a Pt/Activated Carbon Catalyst. Journal of Physical Chemistry C, 2014, 118, 26750-26763.	3.1	20
43	Toward Efficient Drug Delivery through Suitably Prepared Metalâ€“Organic Frameworks: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 8885-8890.	3.1	37
44	Properties and energetics for design and characterization of chitosan nanoparticles used for drug encapsulation. RSC Advances, 2014, 4, 12653.	3.6	18
45	Carbon-Based Nanoporous Networks as Media for the Separation of CO₂/CH₄Mixtures: A Molecular Dynamics Approach. Journal of Physical Chemistry C, 2013, 117, 19373-19381.	3.1	26
46	Atomic Hydrogen Diffusion on Doped and Chemically Modified Graphene. Journal of Physical Chemistry C, 2013, 117, 6312-6319.	3.1	25
47	A cyclam-type â€œturn onâ€•fluorescent sensor selective for mercury ions in aqueous media. RSC Advances, 2012, 2, 12679.	3.6	18
48	Hydrogen Storage in Novel Li-Doped Corrole Metal-Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 8359-8363.	3.1	30
49	Computational Prediction of New Hydrocarbon Materials: The Hydrogenated Forms of Graphdiyne. Journal of Physical Chemistry C, 2012, 116, 19211-19214.	3.1	32
50	Insight on the Formation of Chitosan Nanoparticles through Ionotropic Gelation with Tripolyphosphate. Molecular Pharmaceutics, 2012, 9, 2856-2862.	4.6	177
51	Enhanced hydrogen storage by spillover on metal-doped carbon foam: an experimental and computational study. Nanoscale, 2011, 3, 933.	5.6	65
52	Ab-Initio Study of the Adsorption and Separation of NO_x and SO_x Gases in Functionalized IRMOF Ligands. Journal of Physical Chemistry C, 2011, 115, 24906-24914.	3.1	21
53	Multi-scale theoretical investigation of hydrogen storage in covalent organic frameworks. Nanoscale, 2011, 3, 856.	5.6	88
54	Molecular dynamics simulations of thermal transport in porous nanotube network structures. Nanoscale, 2011, 3, 3679.	5.6	31

#	Article	IF	Citations
55	Theoretical Study of Amino Acid Interaction with Metal Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 272-275.	4.6	16
56	On the Enhancement of Molecular Hydrogen Interactions in Nanoporous Solids for Improved Hydrogen Storage. Journal of Physical Chemistry Letters, 2011, 2, 1824-1830.	4.6	32
57	Theoretical Explanation of Hydrogen Spillover in Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2011, 115, 4047-4053.	3.1	38
58	Hydrogen storage in nanotubes & nanostructures. Materials Today, 2011, 14, 324-328.	14.2	131
59	Li-Doped Pillared Graphene Oxide: A Graphene-Based Nanostructured Material for Hydrogen Storage. Journal of Physical Chemistry Letters, 2010, 1, 2459-2464.	4.6	95
60	Designing 3D COFs with Enhanced Hydrogen Storage Capacity. Nano Letters, 2010, 10, 452-454.	9.1	144
61	Enhancement of Hydrogen Adsorption in Metalâ^'Organic Frameworks by Mg²⁺ Functionalization: A Multiscale Computational Study. Journal of Physical Chemistry C, 2010, 114, 16855-16858.	3.1	31
62	Modeling of Thermal Transport in Pillared-Graphene Architectures. ACS Nano, 2010, 4, 1153-1161.	14.6	280
63	Grand Canonical Monte Carlo Method for Gas Adsorption and Separation. Journal of Computational and Theoretical Nanoscience, 2009, 6, 335-348.	0.4	17
64	Ab initio Study of the Interactions between CO₂ and Nâ€Containing Organic Heterocycles. ChemPhysChem, 2009, 10, 374-383.	2.1	180
65	DFT Study of the Hydrogen Spillover Mechanism on Pt-Doped Graphite. Journal of Physical Chemistry C, 2009, 113, 14908-14915.	3.1	136
66	The effect of structural and energetic parameters of MOFs and COFs towards the improvement of their hydrogen storage properties. Nanotechnology, 2009, 20, 204030.	2.6	32
67	DFT Study of Hydrogen Storage by Spillover on Graphite with Oxygen Surface Groups. Journal of the American Chemical Society, 2009, 131, 15133-15135.	13.7	108
68	Hydrogen Storage in Lithium-Functionalized 3-D Covalent-Organic Framework Materials. Journal of Physical Chemistry C, 2009, 113, 21253-21257.	3.1	68
69	Enhancement of Hydrogen Adsorption in Metalâ^'Organic Frameworks by the Incorporation of the Sulfonate Group and Li Cations. A Multiscale Computational Study. Journal of the American Chemical Society, 2009, 131, 13410-13414.	13.7	79
70	Gas Adsorption and Separation by Employing Grand Canonical Monte Carlo Simulations. , 2009, , .		0
71	First Principles Theoretical Study of the Interaction of Hydrogen with the Ultra-Microporous Materials IRMOF And COF. , 2009, , .		0
72	On the Interaction between Carbon Dioxide and Nanomaterials with High Accuracy ab initio and DFT Calculations. , 2009, , .		0

#	Article	IF	Citations
73	Improving Hydrogen Storage Capacity of MOF by Functionalization of the Organic Linker with Lithium Atoms. Nano Letters, 2008, 8, 1572-1576.	9.1	250
74	Hydrogen Storage in 3D Covalent Organic Frameworks. A Multiscale Theoretical Investigation. Journal of Physical Chemistry C, 2008, 112, 9095-9098.	3.1	108
75	Why Li Doping in MOFs Enhances H₂ Storage Capacity? A Multi-scale Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 7290-7294.	3.1	145
76	Pillared Graphene: A New 3-D Network Nanostructure for Enhanced Hydrogen Storage. Nano Letters, 2008, 8, 3166-3170.	9.1	710
77	Assessing the Density Functional Theory in the Hydrogen Storage Problem. Journal of Nanoscience and Nanotechnology, 2008, 8, 3091-3096.	0.9	6
78	Enhancement of the Ionization-Potential of K and Rb upon Chemisorption on a C60Molecule. Journal of Physical Chemistry C, 2007, 111, 6593-6596.	3.1	5
79	Carbon Nanoscrolls:Â A Promising Material for Hydrogen Storage. Nano Letters, 2007, 7, 1893-1897.	9.1	270
80	Effect of curvature and chirality for hydrogen storage in single-walled carbon nanotubes: A Combined ab initio and Monte Carlo investigation. Journal of Chemical Physics, 2007, 126, 144704.	3.0	45
81	Why boron nitride nanotubes are preferable to carbon nanotubes for hydrogen storage?An ab initio theoretical study. Catalysis Today, 2007, 120, 341-345.	4.4	120
82	Glycine Interaction with Carbon Nanotubes:Â An ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6048-6050.	2.6	38
83	SiC Nanotubes:â€‰ A Novel Material for Hydrogen Storage. Nano Letters, 2006, 6, 1581-1583.	9.1	334
84	Haeckelites: A promising anode material for lithium batteries application. An ab initio and molecular dynamics theoretical study. Applied Physics Letters, 2006, 89, 233125.	3.3	18
85	A Multi Scale Theoretical Study of Li⁺ Interaction with Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 3731-3735.	0.9	16
86	Silicon carbide nanotube tips: Promising materials for atomic force microscopy and/or scanning tunneling microscopy. Applied Physics Letters, 2006, 89, 123126.	3.3	35
87	Why alkali metals preferably bind on structural defects of carbon nanotubes: A theoretical study by first principles. Journal of Chemical Physics, 2006, 125, 204707.	3.0	40
88	Hydrogen storage in carbon nanotubes: a multi-scale theoretical study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	0
89	Carbon-nanotube tips with edge made of a transition metal. Applied Physics Letters, 2005, 87, 193105.	3.3	19
90	Magnetic enhancement and magnetic reduction in binary clusters of transition metal atoms. Journal of Chemical Physics, 2004, 120, 11901-11904.	3.0	31

#	Article	IF	Citations
91	An MRD-CI study of the electronic spectrum of Si3C3. Journal of Molecular Spectroscopy, 2004, 223, 96-100.	1.2	4
92	Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Naâˆ’Y:Â Control of Site Selectivity by Cationâˆ’Arene Interactions. Journal of Organic Chemistry, 2003, 68, 2839-2843.	3.2	17
93	From Pure Carbon to Siliconâˆ’Carbon Nanotubes:â€‰ An Ab-initio Study. Nano Letters, 2003, 3, 1481-1484.	9.1	193
94	Understanding the structure of metal encapsulated Si cages and nanotubes: Role of symmetry and d-band filling. Journal of Chemical Physics, 2003, 119, 7498-7502.	3.0	56
95	Stereochemistry of the [4Â+Â2] Cycloadditions oftrans,trans- andcis,trans-2,4-Hexadiene to C60. Journal of Organic Chemistry, 2002, 67, 3284-3289.	3.2	10
96	Structure and Stability of Ni-Encapsulated Si Nanotube. Nano Letters, 2002, 2, 301-304.	9.1	70
97	Stabilization of Si-based cage clusters and nanotubes by encapsulation of transition metal atoms. New Journal of Physics, 2002, 4, 78-78.	2.9	92
98	The electronic spectrum of linear pentadiynylidene in comparison with isomeric ethynylcyclopropenylidene. Physical Chemistry Chemical Physics, 2002, 4, 3318-3321.	2.8	13
99	Mass spectra and structures of Cu+Rgn clusters (Rg=Ne, Ar). Chemical Physics, 2002, 280, 43-51.	1.9	23
100	Importance of multi-reference configuration interaction for 3Î£uâˆ’â†X3Î£gâˆ’ transitions of linear HC7H. Chemical Physics Letters, 2002, 356, 398-402.	2.6	8
101	Hydrogen interaction with carbon nanotubes: a review of ab initio studies. Journal of Physics Condensed Matter, 2002, 14, R453-R465.	1.8	88
102	Hydrogen Interaction with Single-Walled Carbon Nanotubes:Â A Combined Quantum-Mechanics/Molecular-Mechanics Study. Nano Letters, 2001, 1, 179-182.	9.1	86
103	Why Alkali-Metal-Doped Carbon Nanotubes Possess High Hydrogen Uptake. Nano Letters, 2001, 1, 531-533.	9.1	221
104	Stereochemistry in the Reaction of 4-Methyl-1,2,4-triazoline-3,5-dione (MTAD) with Î²,Î²-Dimethyl-p-methoxystyrene. Are Open Biradicals the Reaction Intermediates?â€. Journal of Organic Chemistry, 2001, 66, 3682-3687.	3.2	25
105	cis- and trans-N-Benzyl-octahydrobenzo[g]quinolines. Adrenergic and Dopaminergic Activity Studies. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 883-886.	2.2	5
106	Theoretical and experimental studies of metallated phenanthroline derivatives as carriers for the optimization of the nitrate sensor. Analytica Chimica Acta, 2001, 439, 273-280.	5.4	16
107	Ab initio CCSD(T) and MRD-CI study of excited states and the electronic spectrum of linear C5+. Chemical Physics Letters, 2001, 340, 559-564.	2.6	13
108	Structural properties of metal-benzene, Mn(benzene)m, M=Ni, V complexes: an ab initio study. Chemical Physics Letters, 2001, 350, 393-398.	2.6	26

#	Article	IF	Citations
109	MRD-CI study of the electronic spectrum of linear C9. Chemical Physics Letters, 2001, 336, 171-176.	2.6	19
110	The electronic spectrum of C11 in its linear and cyclic conformation. Physical Chemistry Chemical Physics, 2001, 3, 3913-3916.	2.8	11
111	Extreme hydrogen sensitivity of the transport properties of single-wall carbon-nanotube capsules. Physical Review B, 2001, 64, .	3.2	24
112	CATALYTIC ACTION OF NI ATOMS IN THE FORMATION OF CARBON NANOTUBES: A COMBINED AB-INITIO AND MOLECULAR DYNAMICS STUDY. , 2001, , .		0
113	Curvature dependence of the metal catalyst atom interaction with carbon nanotubes walls. Chemical Physics Letters, 2000, 320, 425-434.	2.6	151
114	The electronic spectrum of linear and rhombic C4. Chemical Physics Letters, 2000, 324, 195-200.	2.6	25
115	Mass spectra and theoretical modeling of Li+Nen, Li+Arn and Li+Krn clusters. Chemical Physics, 2000, 258, 13-20.	1.9	27
116	Anomalous temperature dependence of the resistivity of single-wall carbon nanotubes. Physical Review B, 2000, 61, R13393-R13396.	3.2	11
117	Various bonding configurations of transition-metal atoms on carbon nanotubes: Their effect on contact resistance. Applied Physics Letters, 2000, 76, 3890-3892.	3.3	73
118	Catalytic Action of Ni Atoms in the Formation of Carbon Nanotubes: A Molecular Dynamics Study. Physical Review Letters, 2000, 85, 3193-3196.	7.8	106
119	Complete Assignment of1H and13C NMR Spectra of Poly(N-vinylcarbazole). Macromolecules, 2000, 33, 3180-3183.	4.8	36
120	Site Specificity in the Photooxidation of Some Trisubstituted Alkenes in Thionin-Supported Zeolite Naâ^'Y. On the Role of the Alkali Metal Cation. Organic Letters, 2000, 2, 1369-1372.	4.6	49
121	Contrasting bonding behaviors of3dtransition metal atoms with graphite andC60. Physical Review B, 2000, 62, 9867-9871.	3.2	38
122	Tight-binding molecular dynamics study of transition metal carbide clusters. Chemical Physics Letters, 1999, 301, 503-508.	2.6	51
123	Coordination of Ti cation embedded in argon clusters. Chemical Physics Letters, 1999, 302, 595-601.	2.6	10
124	Tight-Binding Molecular Dynamics Study of Heteronuclear Systems: Application to Si m Ge n Clusters. Journal of Cluster Science, 1999, 10, 549-556.	3.3	10
125	A tight-binding molecular dynamics study of Ni Si binary clusters. Chemical Physics Letters, 1998, 292, 487-492.	2.6	28
126	Stability and structure of Ni+Arn and Pt+Arn clusters. Journal of Chemical Physics, 1998, 109, 4687-4688.	3.0	21

#	Article	IF	Citations
127	Ab initio study of electronic, structural, and vibrational properties of the Si4C cluster. Journal of Chemical Physics, 1996, 104, 2566-2573.	3.0	26
128	Theoretical study of the Si3C2 cluster. Chemical Physics Letters, 1995, 233, 619-626.	2.6	34
129	Model potential for silicon clusters and surfaces. Physical Review B, 1993, 47, 10648-10653.	3.2	13
130	Reproduction of quantum tight-binding effects in silicon clusters by a four-body classical model. Journal of Physics Condensed Matter, 1993, 5, 6183-6188.	1.8	1