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	Pillared Graphene: A New 3-D Network Nanostructure for Enhanced Hydrogen Storage. Nano Letters, 2008, 8, 3166-3170.	9.1	710
2	Materials for hydrogen-based energy storage â€“ past, recent progress and future outlook. Journal of Alloys and Compounds, 2020, 827, 153548.	5.5	518
3	SiC Nanotubes:â€‰ A Novel Material for Hydrogen Storage. Nano Letters, 2006, 6, 1581-1583.	9.1	334
4	Modeling of Thermal Transport in Pillared-Graphene Architectures. ACS Nano, 2010, 4, 1153-1161.	14.6	280
5	Carbon Nanoscrolls:Â A Promising Material for Hydrogen Storage. Nano Letters, 2007, 7, 1893-1897.	9.1	270
6	Improving Hydrogen Storage Capacity of MOF by Functionalization of the Organic Linker with Lithium Atoms. Nano Letters, 2008, 8, 1572-1576.	9.1	250
7	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
8	Why Alkali-Metal-Doped Carbon Nanotubes Possess High Hydrogen Uptake. Nano Letters, 2001, 1, 531-533.	9.1	221
9	From Pure Carbon to Siliconâ˜Carbon Nanotubes:â€‰ An Ab-initio Study. Nano Letters, 2003, 3, 1481-1484.	9.1	193
10	Reticular Synthesis of HKUST-like tbo-MOFs with Enhanced CH₄ Storage. Journal of the American Chemical Society, 2016, 138, 1568-1574.	13.7	193
11	Ab initio Study of the Interactions between CO₂ and Nâ€Containing Organic Heterocycles. ChemPhysChem, 2009, 10, 374-383.	2.1	180
12	Insight on the Formation of Chitosan Nanoparticles through Ionotropic Gelation with Tripolyphosphate. Molecular Pharmaceutics, 2012, 9, 2856-2862.	4.6	177
13	Curvature dependence of the metal catalyst atom interaction with carbon nanotubes walls. Chemical Physics Letters, 2000, 320, 425-434.	2.6	151
14	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
15	Designing 3D COFs with Enhanced Hydrogen Storage Capacity. Nano Letters, 2010, 10, 452-454.	9.1	144
16	DFT Study of the Hydrogen Spillover Mechanism on Pt-Doped Graphite. Journal of Physical Chemistry C, 2009, 113, 14908-14915.	3.1	136
17	Hydrogen storage in nanotubes & nanostructures. Materials Today, 2011, 14, 324-328.	14.2	131
18	Outlook and challenges for hydrogen storage in nanoporous materials. Applied Physics A: Materials Science and Processing, 2016, 122, 1.	2.3	129

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19	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
20	Hydrogen Storage in 3D Covalent Organic Frameworks. A Multiscale Theoretical Investigation. Journal of Physical Chemistry C, 2008, 112, 9095-9098.	3.1	108
21	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
22	Chemically intuited, large-scale screening of MOFs by machine learning techniques. Npj Computational Materials, 2017, 3, .	8.7	107
23	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
24	A Universal Machine Learning Algorithm for Large-Scale Screening of Materials. Journal of the American Chemical Society, 2020, 142, 3814-3822.	13.7	98
25	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
26	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
27	Hydrogen interaction with carbon nanotubes: a review of ab initio studies. Journal of Physics Condensed Matter, 2002, 14, R453-R465.	1.8	88
28	Multi-scale theoretical investigation of hydrogen storage in covalent organic frameworks. Nanoscale, 2011, 3, 856.	5.6	88
29	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
30	Hydrogen Interaction with Single-Walled Carbon Nanotubes:Â A Combined Quantum-Mechanics/Molecular-Mechanics Study. Nano Letters, 2001, 1, 179-182.	9.1	86
31	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
32	Review of computer simulations on anti-cancer drug delivery in MOFs. Inorganic Chemistry Frontiers, 2018, 5, 1255-1272.	6.0	79
33	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
34	Structure and Stability of Ni-Encapsulated Si Nanotube. Nano Letters, 2002, 2, 301-304.	9.1	70
35	Hydrogen Storage in Lithium-Functionalized 3-D Covalent-Organic Framework Materials. Journal of Physical Chemistry C, 2009, 113, 21253-21257.	3.1	68
36	Enhanced hydrogen storage by spillover on metal-doped carbon foam: an experimental and computational study. Nanoscale, 2011, 3, 933.	5.6	65

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37	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
38	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
39	Tight-binding molecular dynamics study of transition metal carbide clusters. Chemical Physics Letters, 1999, 301, 503-508.	2.6	51
40	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
41	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
42	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
43	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
44	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
45	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
46	Contrasting bonding behaviors of3dtransition metal atoms with graphite andC60. Physical Review B, 2000, 62, 9867-9871.	3.2	38
47	Glycine Interaction with Carbon Nanotubes:Â An ab Initio Study. Journal of Physical Chemistry B, 2006, 110, 6048-6050.	2.6	38
48	Theoretical Explanation of Hydrogen Spillover in Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2011, 115, 4047-4053.	3.1	38
49	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
50	Complete Assignment of1H and13C NMR Spectra of Poly(N-vinylcarbazole). Macromolecules, 2000, 33, 3180-3183.	4.8	36
51	Silicon carbide nanotube tips: Promising materials for atomic force microscopy and/or scanning tunneling microscopy. Applied Physics Letters, 2006, 89, 123126.	3.3	35
52	Theoretical study of the Si3C2 cluster. Chemical Physics Letters, 1995, 233, 619-626.	2.6	34
53	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
54	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

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55	Computational Prediction of New Hydrocarbon Materials: The Hydrogenated Forms of Graphdiyne. Journal of Physical Chemistry C, 2012, 116, 19211-19214.	3.1	32
56	Magnetic enhancement and magnetic reduction in binary clusters of transition metal atoms. Journal of Chemical Physics, 2004, 120, 11901-11904.	3.0	31
57	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
58	Molecular dynamics simulations of thermal transport in porous nanotube network structures. Nanoscale, 2011, 3, 3679.	5.6	31
59	Hydrogen Storage in Novel Li-Doped Corrole Metal-Organic Frameworks. Journal of Physical Chemistry C, 2012, 116, 8359-8363.	3.1	30
60	Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 9825-9829.	7.1	30
61	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
62	Water-stable 2-D Zr MOFs with exceptional UO₂²⁺ sorption capability. Journal of Materials Chemistry A, 2020, 8, 1849-1857.	10.3	29
63	A tight-binding molecular dynamics study of Ni Si binary clusters. Chemical Physics Letters, 1998, 292, 487-492.	2.6	28
64	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
65	Mass spectra and theoretical modeling of Li+Nen, Li+Arn and Li+Krn clusters. Chemical Physics, 2000, 258, 13-20.	1.9	27
66	Ab initio study of electronic, structural, and vibrational properties of the Si4C cluster. Journal of Chemical Physics, 1996, 104, 2566-2573.	3.0	26
67	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
68	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
69	The electronic spectrum of linear and rhombic C4. Chemical Physics Letters, 2000, 324, 195-200.	2.6	25
70	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
71	Atomic Hydrogen Diffusion on Doped and Chemically Modified Graphene. Journal of Physical Chemistry C, 2013, 117, 6312-6319.	3.1	25
72	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

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73	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
74	Extreme hydrogen sensitivity of the transport properties of single-wall carbon-nanotube capsules. Physical Review B, 2001, 64, .	3.2	24
75	Mass spectra and structures of Cu+Rgn clusters (Rg=Ne, Ar). Chemical Physics, 2002, 280, 43-51.	1.9	23
76	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
77	Stability and structure of Ni+Arn and Pt+Arn clusters. Journal of Chemical Physics, 1998, 109, 4687-4688.	3.0	21
78	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
79	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
80	OH-functionalization strategy in Metal-Organic Frameworks for drug delivery. Chemical Physics Letters, 2017, 685, 114-118.	2.6	20
81	MRD-CI study of the electronic spectrum of linear C9. Chemical Physics Letters, 2001, 336, 171-176.	2.6	19
82	Carbon-nanotube tips with edge made of a transition metal. Applied Physics Letters, 2005, 87, 193105.	3.3	19
83	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
84	A cyclam-type â€œturn onâ€•fluorescent sensor selective for mercury ions in aqueous media. RSC Advances, 2012, 2, 12679.	3.6	18
85	Properties and energetics for design and characterization of chitosan nanoparticles used for drug encapsulation. RSC Advances, 2014, 4, 12653.	3.6	18
86	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
87	Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Naâ^'Y:Â Control of Site Selectivity by Cationâ^'Arene Interactions. Journal of Organic Chemistry, 2003, 68, 2839-2843.	3.2	17
88	Grand Canonical Monte Carlo Method for Gas Adsorption and Separation. Journal of Computational and Theoretical Nanoscience, 2009, 6, 335-348.	0.4	17
89	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
90	A Multi Scale Theoretical Study of Li⁺ Interaction with Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2006, 6, 3731-3735.	0.9	16

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91	Theoretical Study of Amino Acid Interaction with Metal Organic Frameworks. Journal of Physical Chemistry Letters, 2011, 2, 272-275.	4.6	16
92	Cryogenic Characterization of FBK RGB-HD SiPMs. Journal of Instrumentation, 2017, 12, P09030-P09030.	1.2	16
93	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
94	Ab Initio Study of the Adsorption of CO₂ on Functionalized Benzenes. ChemPhysChem, 2014, 15, 905-911.	2.1	15
95	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
96	Model potential for silicon clusters and surfaces. Physical Review B, 1993, 47, 10648-10653.	3.2	13
97	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
98	The electronic spectrum of linear pentadiynylidene in comparison with isomeric ethynylcyclopropenylidene. Physical Chemistry Chemical Physics, 2002, 4, 3318-3321.	2.8	13
99	Anomalous temperature dependence of the resistivity of single-wall carbon nanotubes. Physical Review B, 2000, 61, R13393-R13396.	3.2	11
100	The electronic spectrum of C11 in its linear and cyclic conformation. Physical Chemistry Chemical Physics, 2001, 3, 3913-3916.	2.8	11
101	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
102	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
103	Coordination of Ti cation embedded in argon clusters. Chemical Physics Letters, 1999, 302, 595-601.	2.6	10
104	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
105	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
106	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
107	Enhancement of CO₂ Adsorption in Magnesium Alkoxide IRMOF-10. Journal of Physical Chemistry C, 2015, 119, 22001-22007.	3.1	9
108	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

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109	Importance of multi-reference configuration interaction for 3Î£uâ^'â†X3Î£gâ^' transitions of linear HC7H. Chemical Physics Letters, 2002, 356, 398-402.	2.6	8
110	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
111	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
112	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
113	Direct observation of spin-injection in tyrosinate-functionalized single-wall carbon nanotubes. Carbon, 2014, 67, 424-433.	10.3	7
114	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
115	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
116	Linker Functionalization Strategy for Water Adsorption in Metalâ€"Organic Frameworks. Molecules, 2022, 27, 2614.	3.8	7
117	Assessing the Density Functional Theory in the Hydrogen Storage Problem. Journal of Nanoscience and Nanotechnology, 2008, 8, 3091-3096.	0.9	6
118	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
119	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
120	Organically interconnected graphene flakes: A flexible 3-D material with tunable electronic bandgap. Scientific Reports, 2019, 9, 13676.	3.3	5
121	Surface Modification Strategy for Enhanced NO2 Capture in Metalâ€"Organic Frameworks. Molecules, 2022, 27, 3448.	3.8	5
122	An MRD-CI study of the electronic spectrum of Si3C3. Journal of Molecular Spectroscopy, 2004, 223, 96-100.	1.2	4
123	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
124	Enhancing of CO Uptake in Metal-Organic Frameworks by Linker Functionalization: A Multi-Scale Theoretical Study. Chemistry, 2022, 4, 603-614.	2.2	4
125	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
126	Gas Adsorption and Separation by Employing Grand Canonical Monte Carlo Simulations. , 2009, , .		0

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127	First Principles Theoretical Study of the Interaction of Hydrogen with the Ultra-Microporous Materials IRMOF And COF. , 2009, , .		0
128	On the Interaction between Carbon Dioxide and Nanomaterials with High Accuracy ab initio and DFT Calculations. , 2009, , .		0
129	CATALYTIC ACTION OF NI ATOMS IN THE FORMATION OF CARBON NANOTUBES: A COMBINED AB-INITIO AND MOLECULAR DYNAMICS STUDY. , 2001, , .		0
130	Hydrogen storage in carbon nanotubes: a multi-scale theoretical study. Journal of Nanoscience and Nanotechnology, 2006, 6, 87-90.	0.9	0