Jenny G Vitillo

List of Publications by Year
in descending order

96 papers	6,163 citations	81900 39 h-index	69250 77 g-index
100 all docs	100 docs citations	100 times ranked	6966 citing authors

#	Article	IF	Citations
1	Local Structure of Framework Cu(II) in HKUST-1 Metallorganic Framework:Â Spectroscopic Characterization upon Activation and Interaction with Adsorbates. Chemistry of Materials, 2006, 18, 1337-1346.	6.7	647
2	Tuned to Perfection: Ironing Out the Defects in Metalâ€“Organic Framework UiO-66. Chemistry of Materials, 2014, 26, 4068-4071.	6.7	634
3	H₂storage in isostructural UiO-67 and UiO-66 MOFs. Physical Chemistry Chemical Physics, 2012, 14, 1614-1626.	2.8	415
4	Role of Exposed Metal Sites in Hydrogen Storage in MOFs. Journal of the American Chemical Society, 2008, 130, 8386-8396.	13.7	384
5	Liquid Hydrogen in Protonic Chabazite. Journal of the American Chemical Society, 2005, 127, 6361-6366.	13.7	204
6	Local Structure of CPO-27-Ni Metallorganic Framework upon Dehydration and Coordination of NO. Chemistry of Materials, 2008, 20, 4957-4968.	6.7	195
7	Functionalizing the Defects: Postsynthetic Ligand Exchange in the Metal Organic Framework UiO-66. Chemistry of Materials, 2016, 28, 7190-7193.	6.7	170
8	Interaction of Hydrogen with MOF-5. Journal of Physical Chemistry B, 2005, 109, 18237-18242.	2.6	157
9	Introduction: Carbon Capture and Separation. Chemical Reviews, 2017, 117, 9521-9523.	47.7	157
10	CO Adsorption on CPO-27-Ni Coordination Polymer: Spectroscopic Features and Interaction Energy. Journal of Physical Chemistry C, 2009, 113, 3292-3299.	3.1	121
11	Functionalization of UiO-66 Metalâˆ’Organic Framework and Highly Cross-Linked Polystyrene with Cr(CO)₃: In Situ Formation, Stability, and Photoreactivity. Chemistry of Materials, 2010, 22, 4602-4611.	6.7	120
12	Theoretical maximal storage of hydrogen in zeolitic frameworks. Physical Chemistry Chemical Physics, 2005, 7, 3948.	2.8	102
13	Hydrogen storage in Chabazite zeolite frameworks. Physical Chemistry Chemical Physics, 2005, 7, 3197.	2.8	100
14	Response of CPO-27-Ni towards CO, N2 and C2H4. Physical Chemistry Chemical Physics, 2009, 11, 9811.	2.8	87
15	Carbon Dioxide Adsorption in Amineâ€Functionalized Mixedâ€Ligand Metalâ€“Organic Frameworks of UiOâ€66 Topology. ChemSusChem, 2014, 7, 3382-3388.	6.8	83
16	Quantum Chemical Characterization of Structural Single Fe(II) Sites in MIL-Type Metalâ€“Organic Frameworks for the Oxidation of Methane to Methanol and Ethane to Ethanol. ACS Catalysis, 2019, 9, 2870-2879.	11.2	82
17	Nanoporous Crystalline Phases of Poly(2,6-Dimethyl-1,4-phenylene)oxide. Chemistry of Materials, 2011, 23, 3195-3200.	6.7	81
18	Structure, Dynamics, and Reactivity for Light Alkane Oxidation of Fe(II) Sites Situated in the Nodes of a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 18142-18151.	13.7	80

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19	Theoretical characterization of dihydrogen adducts with alkaline cations. Journal of Chemical Physics, 2005, 122, 114311.	3.0	79
20	Cyclodextrin nanosponges as effective gas carriers. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2011, 71, 189-194.	1.6	72
21	Structureâ€“activity relationships of simple molecules adsorbed on CPO-27-Ni metalâ€“organic framework: In situ experiments vs. theory. Catalysis Today, 2012, 182, 67-79.	4.4	67
22	Coreâ€“Shell Structure of Palladium Hydride Nanoparticles Revealed by Combined X-ray Absorption Spectroscopy and X-ray Diffraction. Journal of Physical Chemistry C, 2017, 121, 18202-18213.	3.1	67
23	Tailoring Metalâ€“Organic Frameworks for CO₂ Capture: The Amino Effect. ChemSusChem, 2011, 4, 1281-1290.	6.8	66
24	Magnesium-based systems for carbon dioxide capture, storage and recycling: from leaves to synthetic nanostructured materials. RSC Advances, 2015, 5, 36192-36239.	3.6	61
25	CO₂ Capture in Dry and Wet Conditions in UTSA-16 Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2017, 9, 455-463.	8.0	61
26	Direct evidence of adsorption induced CrII mobility on the SiO₂surface upon complexation by CO. Chemical Communications, 2010, 46, 976-978.	4.1	59
27	Design of high surface area poly(ionic liquid)s to convert carbon dioxide into ethylene carbonate. Journal of Materials Chemistry A, 2015, 3, 8508-8518.	10.3	58
28	New insights into UTSA-16. Physical Chemistry Chemical Physics, 2016, 18, 220-227.	2.8	56
29	Structure and Thermodynamic Properties of the NaMgH₃ Perovskite: A Comprehensive Study. Chemistry of Materials, 2011, 23, 2317-2326.	6.7	54
30	Beyond Radical Rebound: Methane Oxidation to Methanol Catalyzed by Iron Species in Metalâ€“Organic Framework Nodes. Journal of the American Chemical Society, 2021, 143, 12165-12174.	13.7	51
31	Aerogels and Polymorphism of Isotactic Poly(4-methyl-pentene-1). ACS Applied Materials & Interfaces, 2011, 3, 969-977.	8.0	49
32	Solventâ€Driven Gate Opening in MOFâ€76â€Ce: Effect on CO₂ Adsorption. ChemSusChem, 2016, 9, 713-719.	6.8	49
33	Hydrogen uptake and diffusion in Callovo-Oxfordian clay rock for nuclear waste disposal technology. Applied Geochemistry, 2014, 49, 168-177.	3.0	48
34	Interaction of H2with Alkali-Metal-Exchanged Zeolites:â€‰ a Quantum Mechanical Study. Journal of Physical Chemistry C, 2007, 111, 2505-2513.	3.1	47
35	FTIR spectroscopy and thermodynamics of CO and H2 adsorbed on Î³-, Î´- and Î±-Al2O3. Physical Chemistry Chemical Physics, 2010, 12, 6474.	2.8	47
36	Time-resolved operando studies of carbon supported Pd nanoparticles under hydrogenation reactions by X-ray diffraction and absorption. Faraday Discussions, 2018, 208, 187-205.	3.2	47

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37	Hydrogen Adsorption by Î´ and Îµ Crystalline Phases of Syndiotactic Polystyrene Aerogels. Macromolecules, 2010, 43, 8594-8601.	4.8	42
38	Close-Packed Dye Molecules in Zeolite Channels Self-Assemble into Supramolecular Nanoladders. Journal of Physical Chemistry C, 2014, 118, 15732-15743.	3.1	41
39	Monolithic nanoporousâ€"crystalline aerogels based on PPO. RSC Advances, 2012, 2, 12011.	3.6	40
40	FTIR spectroscopy and thermodynamics of hydrogen adsorbed in a cross-linked polymer. Physical Chemistry Chemical Physics, 2007, 9, 4992.	2.8	38
41	Oriented TiO₂ Nanostructured Pillar Arrays: Synthesis and Characterization. Advanced Materials, 2008, 20, 3342-3348.	21.0	38
42	Hydrogen adsorption and diffusion in synthetic Na-montmorillonites at high pressures and temperature. International Journal of Hydrogen Energy, 2015, 40, 2698-2709.	7.1	38
43	Crystal structure refinement of a sepiolite/indigo Maya Blue pigment using molecular modelling and synchrotron diffraction. European Journal of Mineralogy, 2011, 23, 449-466.	1.3	36
44	Understanding and Controlling the Dielectric Response of Metalâ€"Organic Frameworks. ChemPlusChem, 2018, 83, 308-316.	2.8	36
45	Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€"organic framework. Nature Communications, 2020, 11, 3087.	12.8	36
46	Preparation and adsorption properties of activated porous carbons obtained using volatile zinc templating phases. Carbon, 2012, 50, 2047-2051.	10.3	35
47	Spectroscopic and Structural Characterization of Thermal Decomposition of Î³-Mg(BH₄)₂: Dynamic Vacuum versus H₂ Atmosphere. Journal of Physical Chemistry C, 2015, 119, 25340-25351.	3.1	35
48	Conductive ZSM-5-Based Adsorbent for CO₂ Capture: Active Phase vs Monolith. Industrial & Engineering Chemistry Research, 2017, 56, 8485-8498.	3.7	35
49	Influence of First and Second Coordination Environment on Structural Fe(II) Sites in MIL-101 for Câ€"H Bond Activation in Methane. ACS Catalysis, 2021, 11, 579-589.	11.2	35
50	Silica-supported Ti chloride tetrahydrofuranates, precursors of Zieglerâ€"Natta catalysts. Dalton Transactions, 2013, 42, 12706.	3.3	33
51	Evolution and Reversibility of Host/Guest Interactions with Temperature Changes in a Methyl Red@Palygorskite Polyfunctional Hybrid Nanocomposite. Journal of Physical Chemistry C, 2014, 118, 19322-19337.	3.1	33
52	A Multitechnique Approach to Spin-Flips for Cp2Cr(II) Chemistry in Confined State. Journal of Physical Chemistry C, 2010, 114, 4451-4458.	3.1	32
53	Exploring the Chemistry of Electron-Accepting Molecules in the Cavities of the Basic Microporous P4VP Polymer by in situ FTIR Spectroscopy. Journal of Physical Chemistry C, 2008, 112, 19493-19500.	3.1	30
54	Storage of hydrogen as a guest of a nanoporous polymeric crystalline phase. Physical Chemistry Chemical Physics, 2010, 12, 5369.	2.8	30

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55	Increasing the stability of Mg₂(dobpdc) metalâ€“organic framework in air through solvent removal. Materials Chemistry Frontiers, 2017, 1, 444-448.	5.9	30
56	Structure and Enhanced Reactivity of Chromocene Carbonyl Confined inside Cavities of NaY Zeolite. Journal of Physical Chemistry C, 2009, 113, 7305-7315.	3.1	29
57	Combined X-ray and Raman Studies on the Effect of Cobalt Additives on the Decomposition of Magnesium Borohydride. Energies, 2015, 8, 9173-9190.	3.1	28
58	Theoretical and experimental study on Mg(BH4)2â€“Zn(BH4)2 mixed borohydrides. Journal of Alloys and Compounds, 2013, 580, S282-S286.	5.5	27
59	Stability and Reactivity of Grafted Cr(CO)3Species on MOF Linkers: A Computational Study. Inorganic Chemistry, 2009, 48, 5439-5448.	4.0	26
60	Fast carbon dioxide recycling by reaction with Î³-Mg(BH₄)₂. Physical Chemistry Chemical Physics, 2014, 16, 22482-22486.	2.8	26
61	A multi-technique approach to disclose the reaction mechanism of dimethyl carbonate synthesis over amino-modified SBA-15 catalysts. Applied Catalysis B: Environmental, 2017, 211, 323-336.	20.2	26
62	Spectroscopic and adsorptive studies of a thermally robust pyrazolato-based PCP. Dalton Transactions, 2012, 41, 4012.	3.3	25
63	CO₂ Adsorption Sites in UTSA-16: Multitechnique Approach. Journal of Physical Chemistry C, 2016, 120, 12068-12074.	3.1	23
64	Material properties and empirical rate equations for hydrogen sorption reactions in 2 LiNH2â€“1.1 MgH2â€“0.1 LiBH4â€“3Âwt.% ZrCoH3. International Journal of Hydrogen Energy, 2014, 39, 8283-8292.	7.1	22
65	Structure and Hostâ€“Guest Interactions of Peryleneâ€“Diimide Dyes in Zeolite L Nanochannels. Journal of Physical Chemistry C, 2018, 122, 3401-3418.	3.1	22
66	The role of carbon capture, utilization, and storage for economic pathways that limit global warming to below 1.5Â°C. IScience, 2022, 25, 104237.	4.1	22
67	Theoretical characterization of dihydrogen adducts with halide anions. Journal of Chemical Physics, 2006, 124, 224308.	3.0	21
68	Modeling CO and N₂Adsorption at Cr Surface Species of Phillips Catalyst by Hybrid Density Functionals: Effect of Hartreeâ^'Fock Exchange Percentage. Journal of Physical Chemistry A, 2009, 113, 14261-14269.	2.5	21
69	Hydrogen Uptake by {H[Mg(HCOO)₃]âŠƒNHMe₂}_{â^ž} and Determination of Its H₂ Adsorption Sites through Monte Carlo Simulations. Langmuir, 2011, 27, 10124-10131.	3.5	21
70	Direct observation and modelling of ordered hydrogen adsorption and catalyzed orthoâ€“para conversion on ETS-10 titanosilicate material. Physical Chemistry Chemical Physics, 2007, 9, 2753-2760.	2.8	20
71	Characterization of MOFs. 1. Combined Vibrational and Electronic Spectroscopies. RSC Catalysis Series, 2013, , 76-142.	0.1	20
72	Looking for the active hydrogen species in a 5Âwt% Pt/C catalyst: a challenge for inelastic neutron scattering. Faraday Discussions, 2018, 208, 227-242.	3.2	20

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73	Thionine Dye Confined in Zeolite L: Synthesis Location and Optical Properties. Journal of Physical Chemistry C, 2015, 119, 16156-16165.	3.1	19
74	Plate-like zinc oxide microcrystals: Synthesis and characterization of a material active toward hydrogen adsorption. Catalysis Today, 2006, 116, 433-438.	4.4	18
75	Chromocene in porous polystyrene: an example of organometallic chemistry in confined spaces. Physical Chemistry Chemical Physics, 2009, 11, 2218.	2.8	17
76	Characterization and Modeling of Reversible CO₂ Capture from Wet Streams by a MgO/Zeolite Y Nanocomposite. Journal of Physical Chemistry C, 2019, 123, 17214-17224.	3.1	17
77	Modeling Metal Influence on the Gate Opening in ZIF-8 Materials. Chemistry of Materials, 2021, 33, 4465-4473.	6.7	17
78	Visible-Light-Driven Photocatalytic Coupling of Benzylamine over Titanium-Based MIL-125-NH2 Metalâ€“Organic Framework: A Mechanistic Study. Journal of Physical Chemistry C, 2020, 124, 23707-23715.	3.1	16
79	Functionalization of CPO-27-Ni through metal hexacarbonyls: The role of open Ni2+ sites. Microporous and Mesoporous Materials, 2012, 157, 56-61.	4.4	13
80	An alternative pathway for the synthesis of isocyanato- and urea-functionalised metalâ€“organic frameworks. Dalton Transactions, 2013, 42, 8249.	3.3	13
81	Monolithic Aerogels Based on Poly(2,6-diphenyl-1,4-phenylene oxide) and Syndiotactic Polystyrene. ACS Applied Materials & Interfaces, 2013, 5, 5493-5499.	8.0	13
82	Role of extraframework metal sites for hydrogen adsorption into the pores of a zeolite: FT-IR study. International Journal of Hydrogen Energy, 2011, 36, 7944-7950.	7.1	12
83	Soft synthesis of isocyanate-functionalised metalâ€“organic frameworks. Dalton Transactions, 2012, 41, 14236.	3.3	12
84	Thermal Treatment Effect on CO and NO Adsorption on Fe(II) and Fe(III) Species in Fe₃O-Based MIL-Type Metalâ€“Organic Frameworks: A Density Functional Theory Study. Inorganic Chemistry, 2021, 60, 11813-11824.	4.0	11
85	Effect of Pore Size, Solvation, and Defectivity on the Perturbation of Adsorbates in MOFs: The Paradigmatic Mg₂(dobpdc) Case Study. Journal of Physical Chemistry C, 2017, 121, 22762-22772.	3.1	9
86	ZIF-8 as a Catalyst in Ethylene Oxide and Propylene Oxide Reaction with CO2 to Cyclic Organic Carbonates. ChemEngineering, 2019, 3, 60.	2.4	8
87	Water-Driven Structural Transformation in Cobalt Trimesate Metal-Organic Frameworks. Energies, 2021, 14, 4751.	3.1	8
88	On the structure of superbasic (MgO)_n sites solvated in a faujasite zeolite. Physical Chemistry Chemical Physics, 2018, 20, 18503-18514.	2.8	7
89	Multireference Methods are Realistic and Useful Tools for Modeling Catalysis. Israel Journal of Chemistry, 2022, 62, .	2.3	6
90	Low temperature activation and reactivity of CO2 over a CrII-based heterogeneous catalyst: a spectroscopic study. Physical Chemistry Chemical Physics, 2012, 14, 6538.	2.8	5

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91	The role of surfaces in hydrogen storage. Studies in Surface Science and Catalysis, 2005, 155, 481-492.	1.5	4
92	Experimental and computational characterization of phase transitions in CsB3H8. Physical Chemistry Chemical Physics, 2021, 23, 17836-17847.	2.8	4
93	Hydrogen Storage in Chabazite Zeolite Frameworks.. ChemInform, 2005, 36, no.	0.0	1
94	Liquid Hydrogen in Protonic Chabazite.. ChemInform, 2005, 36, no.	0.0	0
95	News and analysis on materials solutions to energy challenges. MRS Bulletin, 2011, 36, 963-963.	3.5	0
96	Effective transport of electronic excitation energy through zeolite channels: a structural study. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s300-s300.	0.1	0