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	Multireference Methods are Realistic and Useful Tools for Modeling Catalysis. Israel Journal of Chemistry, 2022, 62, .	2.3	6
2	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
3	Experimental and computational characterization of phase transitions in CsB3H8. Physical Chemistry Chemical Physics, 2021, 23, 17836-17847.	2.8	4
4	Modeling Metal Influence on the Gate Opening in ZIF-8 Materials. Chemistry of Materials, 2021, 33, 4465-4473.	6.7	17
5	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
6	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
7	Water-Driven Structural Transformation in Cobalt Trimesate Metal-Organic Frameworks. Energies, 2021, 14, 4751.	3.1	8
8	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
9	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
10	Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€“organic framework. Nature Communications, 2020, 11, 3087.	12.8	36
11	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
12	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
13	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
14	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
15	Understanding and Controlling the Dielectric Response of Metalâ€“Organic Frameworks. ChemPlusChem, 2018, 83, 308-316.	2.8	36
16	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
17	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
18	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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19	On the structure of superbasic (MgO)_n sites solvated in a faujasite zeolite. Physical Chemistry Chemical Physics, 2018, 20, 18503-18514.	2.8	7
20	CO₂ Capture in Dry and Wet Conditions in UTSA-16 Metalâ€“Organic Framework. ACS Applied Materials & Interfaces, 2017, 9, 455-463.	8.0	61
21	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
22	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
23	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
24	Introduction: Carbon Capture and Separation. Chemical Reviews, 2017, 117, 9521-9523.	47.7	157
25	Conductive ZSM-5-Based Adsorbent for CO₂ Capture: Active Phase vs Monolith. Industrial & Engineering Chemistry Research, 2017, 56, 8485-8498.	3.7	35
26	Increasing the stability of Mg₂(dobpdc) metalâ€“organic framework in air through solvent removal. Materials Chemistry Frontiers, 2017, 1, 444-448.	5.9	30
27	Solventâ€Driven Gate Opening in MOFâ€76â€Ce: Effect on CO₂ Adsorption. ChemSusChem, 2016, 9, 713-719.	6.8	49
28	Functionalizing the Defects: Postsynthetic Ligand Exchange in the Metal Organic Framework UiO-66. Chemistry of Materials, 2016, 28, 7190-7193.	6.7	170
29	CO₂ Adsorption Sites in UTSA-16: Multitechnique Approach. Journal of Physical Chemistry C, 2016, 120, 12068-12074.	3.1	23
30	New insights into UTSA-16. Physical Chemistry Chemical Physics, 2016, 18, 220-227.	2.8	56
31	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
32	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
33	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
34	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
35	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
36	Thionine Dye Confined in Zeolite L: Synthesis Location and Optical Properties. Journal of Physical Chemistry C, 2015, 119, 16156-16165.	3.1	19

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37	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
38	Tuned to Perfection: Ironing Out the Defects in Metalâ€“Organic Framework UiO-66. Chemistry of Materials, 2014, 26, 4068-4071.	6.7	634
39	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
40	Carbon Dioxide Adsorption in Amineâ€Functionalized Mixedâ€Ligand Metalâ€“Organic Frameworks of UiOâ€66 Topology. ChemSusChem, 2014, 7, 3382-3388.	6.8	83
41	Close-Packed Dye Molecules in Zeolite Channels Self-Assemble into Supramolecular Nanoladders. Journal of Physical Chemistry C, 2014, 118, 15732-15743.	3.1	41
42	Fast carbon dioxide recycling by reaction with Î³-Mg(BH₄)₂. Physical Chemistry Chemical Physics, 2014, 16, 22482-22486.	2.8	26
43	Hydrogen uptake and diffusion in Callovo-Oxfordian clay rock for nuclear waste disposal technology. Applied Geochemistry, 2014, 49, 168-177.	3.0	48
44	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
45	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
46	An alternative pathway for the synthesis of isocyanato- and urea-functionalised metalâ€“organic frameworks. Dalton Transactions, 2013, 42, 8249.	3.3	13
47	Silica-supported Ti chloride tetrahydrofuranates, precursors of Zieglerâ€“Natta catalysts. Dalton Transactions, 2013, 42, 12706.	3.3	33
48	Characterization of MOFs. 1. Combined Vibrational and Electronic Spectroscopies. RSC Catalysis Series, 2013, , 76-142.	0.1	20
49	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
50	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
51	Spectroscopic and adsorptive studies of a thermally robust pyrazolato-based PCP. Dalton Transactions, 2012, 41, 4012.	3.3	25
52	Soft synthesis of isocyanate-functionalised metalâ€“organic frameworks. Dalton Transactions, 2012, 41, 14236.	3.3	12
53	H₂storage in isostructural UiO-67 and UiO-66 MOFs. Physical Chemistry Chemical Physics, 2012, 14, 1614-1626.	2.8	415
54	Monolithic nanoporousâ€“crystalline aerogels based on PPO. RSC Advances, 2012, 2, 12011.	3.6	40

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55	Preparation and adsorption properties of activated porous carbons obtained using volatile zinc templating phases. Carbon, 2012, 50, 2047-2051.	10.3	35
56	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
57	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
58	Nanoporous Crystalline Phases of Poly(2,6-Dimethyl-1,4-phenylene)oxide. Chemistry of Materials, 2011, 23, 3195-3200.	6.7	81
59	Structure and Thermodynamic Properties of the NaMgH₃ Perovskite: A Comprehensive Study. Chemistry of Materials, 2011, 23, 2317-2326.	6.7	54
60	Aerogels and Polymorphism of Isotactic Poly(4-methyl-pentene-1). ACS Applied Materials & Interfaces, 2011, 3, 969-977.	8.0	49
61	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
62	News and analysis on materials solutions to energy challenges. MRS Bulletin, 2011, 36, 963-963.	3.5	0
63	Hydrogen Uptake by {H[Mg(HCOO)₃]âŠƒNHMe₂}_{âˆž} and Determination of Its H₂ Adsorption Sites through Monte Carlo Simulations. Langmuir, 2011, 27, 10124-10131.	3.5	21
64	Cyclodextrin nanosponges as effective gas carriers. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2011, 71, 189-194.	1.6	72
65	Tailoring Metalâ€“Organic Frameworks for CO₂ Capture: The Amino Effect. ChemSusChem, 2011, 4, 1281-1290.	6.8	66
66	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
67	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
68	Hydrogen Adsorption by Î´ and Îµ Crystalline Phases of Syndiotactic Polystyrene Aerogels. Macromolecules, 2010, 43, 8594-8601.	4.8	42
69	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
70	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
71	Direct evidence of adsorption induced CrII mobility on the SiO₂surface upon complexation by CO. Chemical Communications, 2010, 46, 976-978.	4.1	59
72	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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73	Stability and Reactivity of Grafted Cr(CO)3Species on MOF Linkers: A Computational Study. Inorganic Chemistry, 2009, 48, 5439-5448.	4.0	26
74	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
75	Modeling CO and N₂Adsorption at Cr Surface Species of Phillips Catalyst by Hybrid Density Functionals: Effect of Hartreeâˆ’Fock Exchange Percentage. Journal of Physical Chemistry A, 2009, 113, 14261-14269.	2.5	21
76	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
77	Response of CPO-27-Ni towards CO, N2 and C2H4. Physical Chemistry Chemical Physics, 2009, 11, 9811.	2.8	87
78	Chromocene in porous polystyrene: an example of organometallic chemistry in confined spaces. Physical Chemistry Chemical Physics, 2009, 11, 2218.	2.8	17
79	Oriented TiO₂ Nanostructured Pillar Arrays: Synthesis and Characterization. Advanced Materials, 2008, 20, 3342-3348.	21.0	38
80	Role of Exposed Metal Sites in Hydrogen Storage in MOFs. Journal of the American Chemical Society, 2008, 130, 8386-8396.	13.7	384
81	Local Structure of CPO-27-Ni Metallorganic Framework upon Dehydration and Coordination of NO. Chemistry of Materials, 2008, 20, 4957-4968.	6.7	195
82	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
83	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
84	FTIR spectroscopy and thermodynamics of hydrogen adsorbed in a cross-linked polymer. Physical Chemistry Chemical Physics, 2007, 9, 4992.	2.8	38
85	Interaction of H2with Alkali-Metal-Exchanged Zeolites:â€‰ a Quantum Mechanical Study. Journal of Physical Chemistry C, 2007, 111, 2505-2513.	3.1	47
86	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
87	Plate-like zinc oxide microcrystals: Synthesis and characterization of a material active toward hydrogen adsorption. Catalysis Today, 2006, 116, 433-438.	4.4	18
88	Theoretical characterization of dihydrogen adducts with halide anions. Journal of Chemical Physics, 2006, 124, 224308.	3.0	21
89	The role of surfaces in hydrogen storage. Studies in Surface Science and Catalysis, 2005, 155, 481-492.	1.5	4
90	Liquid Hydrogen in Protonic Chabazite. Journal of the American Chemical Society, 2005, 127, 6361-6366.	13.7	204

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91	Liquid Hydrogen in Protonic Chabazite.. ChemInform, 2005, 36, no.	0.0	0
92	Hydrogen Storage in Chabazite Zeolite Frameworks.. ChemInform, 2005, 36, no.	0.0	1
93	Theoretical characterization of dihydrogen adducts with alkaline cations. Journal of Chemical Physics, 2005, 122, 114311.	3.0	79
94	Theoretical maximal storage of hydrogen in zeolitic frameworks. Physical Chemistry Chemical Physics, 2005, 7, 3948.	2.8	102
95	Hydrogen storage in Chabazite zeolite frameworks. Physical Chemistry Chemical Physics, 2005, 7, 3197.	2.8	100
96	Interaction of Hydrogen with MOF-5. Journal of Physical Chemistry B, 2005, 109, 18237-18242.	2.6	157