Gloria Tabacchi

List of Publications by Year
in descending order

92 papers	3,675 citations	126858 33 h-index	138417 58 g-index
120 all docs	120 docs citations	120 times ranked	3253 citing authors

#	Article	IF	Citations
1	A versatile Fe(II) diketonate diamine adduct: Preparation, characterization and validation in the chemical vapor deposition of iron oxide nanomaterials. Materials Chemistry and Physics, 2022, 277, 125534.	2.0	7
2	Spontaneous polymerization of benzofulvene derivatives bearing complexed or un-complexed pyridine rings. European Polymer Journal, 2022, 169, 111137.	2.6	3
3	Facile preparation of a cobalt diamine diketonate adduct as a potential vapor phase precursor for Co₃O₄films. Dalton Transactions, 2021, 50, 10374-10385.	1.6	9
4	Steering polymer growth by molding nanochannels: 1,5-hexadiene polymerization in high silica mordenite. Microporous and Mesoporous Materials, 2021, 311, 110728.	2.2	7
5	A post-HF approach to the sunscreen octyl methoxycinnamate. Journal of Chemical Physics, 2021, 154, 144304.	1.2	3
6	Chemically Induced Mismatch of Rings and Stations in [3]Rotaxanes. Journal of the American Chemical Society, 2021, 143, 8046-8055.	6.6	15
7	The Early Steps of Molecule-to-Material Conversion in Chemical Vapor Deposition (CVD): A Case Study. Molecules, 2021, 26, 1988.	1.7	9
8	Engineering Au/MnO₂ hierarchical nanoarchitectures for ethanol electrochemical valorization. Journal of Materials Chemistry A, 2020, 8, 16902-16907.	5.2	18
9	Precision Molecular Threading/Dethreading. Angewandte Chemie, 2020, 132, 14935-14944.	1.6	10
10	Precision Molecular Threading/Dethreading. Angewandte Chemie - International Edition, 2020, 59, 14825-14834.	7.2	32
11	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	1.2	1,371
12	High-silica mordenite as scaffold for phenylacetylene polymerization: In situ high pressure investigation. Microporous and Mesoporous Materials, 2020, 300, 110163.	2.2	4
13	The Case of Formic Acid on Anatase TiO 2 (101): Where is the Acid Proton?. Angewandte Chemie, 2019, 131, 12561-12564.	1.6	10
14	Confining a Protein-Containing Water Nanodroplet inside Silica Nanochannels. International Journal of Molecular Sciences, 2019, 20, 2965.	1.8	7
15	The Case of Formic Acid on Anatase TiO₂(101): Where is the Acid Proton?. Angewandte Chemie - International Edition, 2019, 58, 12431-12434.	7.2	59
16	Titelbild: The Case of Formic Acid on Anatase TiO₂(101): Where is the Acid Proton? (Angew.) Tj ETQq0 0 0 rgBT /Overlock 1	1.6	1
17	Sensing Nitrogen Mustard Gas Simulant at the ppb Scale via Selective Dual-Site Activation at Au/Mn₃O₄ Interfaces. ACS Applied Materials & Interfaces, 2019, 11, 23692-23700.	4.0	26
18	Differential penetration of ethanol and water in Si-chabazite: High pressure dehydration of azeotrope solution. Microporous and Mesoporous Materials, 2019, 284, 161-169.	2.2	15

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19	Water in zeolite L and its MOF mimic. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 495-511.	0.4	10
20	Computer modeling of apparently straight bond angles: The intriguing case of all-silica ferrierite. American Mineralogist, 2019, 104, 1546-1555.	0.9	8
21	Structure and Hostâ€“Guest Interactions of Peryleneâ€“Diimide Dyes in Zeolite L Nanochannels. Journal of Physical Chemistry C, 2018, 122, 3401-3418.	1.5	22
22	Manganese(II) Molecular Sources for Plasma-Assisted CVD of Mn Oxides and Fluorides: From Precursors to Growth Process. Journal of Physical Chemistry C, 2018, 122, 1367-1375.	1.5	34
23	The effect of pressure on open-framework silicates: elastic behaviour and crystalâ€“fluid interaction. Physics and Chemistry of Minerals, 2018, 45, 115-138.	0.3	44
24	Supramolecular Organization in Confined Nanospaces. ChemPhysChem, 2018, 19, 1249-1297.	1.0	60
25	Unravelling the High-Pressure Behaviour of Dye-Zeolite L Hybrid Materials. Crystals, 2018, 8, 79.	1.0	15
26	Does the Abiotic Formation of Oligopeptides on TiO₂ Nanoparticles Require Special Catalytic Sites? Apparently Not. Journal of Nanoscience and Nanotechnology, 2018, 18, 5854-5857.	0.9	5
27	Irreversible Conversion of a Waterâ€“Ethanol Solution into an Organized Twoâ€Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure. Angewandte Chemie, 2017, 129, 2137-2141.	1.6	6
28	Irreversible Conversion of a Waterâ€“Ethanol Solution into an Organized Twoâ€Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure. Angewandte Chemie - International Edition, 2017, 56, 2105-2109.	7.2	33
29	Structural modification of gallium lanthanum sulfide glass induced by ultrafast laser inscription. , 2017, , .		0
30	Titelbild: Irreversible Conversion of a Waterâ€“Ethanol Solution into an Organized Twoâ€Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure (Angew. Chem.) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.6	0
31	Molecular Engineering of Mn^{II} Diamine Diketonate Precursors for the Vapor Deposition of Manganese Oxide Nanostructures. Chemistry - A European Journal, 2017, 23, 17954-17963.	1.7	33
32	Pressure-Induced Penetration of Water-Ethanol Mixtures in All-Silica Ferrierite. Advanced Science Letters, 2017, 23, 5966-5969.	0.2	8
33	One-dimensional self-assembly of perylene-diimide dyes by unidirectional transit of zeolite channel openings. Chemical Communications, 2016, 52, 11195-11198.	2.2	33
34	Dethreading of a Photoactive Azobenzeneâ€Containing Molecular Axle from a Crown Ether Ring: A Computational Investigation. ChemPhysChem, 2016, 17, 1913-1919.	1.0	17
35	On the Simple Complexity of Carbon Monoxide on Oxide Surfaces: Facetâ€Specific Donation and Backdonation Effects Revealed on TiO₂ Anatase Nanoparticles. ChemPhysChem, 2016, 17, 1956-1960.	1.0	28
36	Behaviour at high pressure of Rb7NaGa8Si12O40Â·3H2O (a zeolite with EDI topology): a combined experimentalâ€“computational study. Physics and Chemistry of Minerals, 2016, 43, 209-216.	0.3	12

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37	Effective transport of electronic excitation energy through zeolite channels: a structural study. Acta Crystallographica Section A: Foundations and Advances, 2015, 71, s300-s300.	0.0	0
38	Structure of Nanochannel Entrances in Stopcockâ€Functionalized Zeoliteâ€...L Composites. Angewandte Chemie - International Edition, 2015, 54, 11112-11116.	7.2	38
39	Opening the Pandora's jar of molecule-to-material conversion in chemical vapor deposition: Insights from theory. International Journal of Quantum Chemistry, 2014, 114, 1-7.	1.0	20
40	CVD precursors for transition metal oxide nanostructures: molecular properties, surface behavior and temperature effects. Physica Status Solidi (A) Applications and Materials Science, 2014, 211, 251-259.	0.8	24
41	Close-Packed Dye Molecules in Zeolite Channels Self-Assemble into Supramolecular Nanoladders. Journal of Physical Chemistry C, 2014, 118, 15732-15743.	1.5	41
42	HP-induced supra-molecular organization of guest molecules in FER-type zeolites. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1469-C1469.	0.0	0
43	Shape-controlled TiO2nanoparticles and TiO2P25 interacting with CO and H2O2molecular probes: a synergic approach for surface structure recognition and physico-chemical understanding. Physical Chemistry Chemical Physics, 2013, 15, 307-315.	1.3	65
44	Surface features of TiO2 nanoparticles: combination modes of adsorbed CO probe the stepping of (101) facets. Physical Chemistry Chemical Physics, 2013, 15, 13391.	1.3	28
45	First-principles simulation of the absorption bands of fluorenone in zeolite L. Physical Chemistry Chemical Physics, 2013, 15, 159-167.	1.3	38
46	Hostâ€“Guest Interactions and Orientation of Dyes in the One-Dimensional Channels of Zeolite L. Langmuir, 2013, 29, 9188-9198.	1.6	44
47	Disentangling proteinâ€“silica interactions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1463-1477.	1.6	11
48	Î²-Fe₂O₃nanomaterials from an iron(<scp>ii</scp>) diketonate-diamine complex: a study from molecular precursor to growth process. Dalton Transactions, 2012, 41, 149-155.	1.6	63
49	Orientation and Order of Xanthene Dyes in the One-Dimensional Channels of Zeolite L: Bridging the Gap between Experimental Data and Molecular Behavior. Journal of Physical Chemistry C, 2012, 116, 16784-16799.	1.5	44
50	An iron(II) diamine diketonate molecular complex: Synthesis, characterization and application in the CVD of Fe2O3 thin films. Inorganica Chimica Acta, 2012, 380, 161-166.	1.2	40
51	How Does Cu^{II} Convert into Cu^I? An Unexpected Ringâ€Mediated Singleâ€Electron Reduction. Chemistry - A European Journal, 2011, 17, 10864-10870.	1.7	31
52	On the Compatibility Criteria for Protein Encapsulation inside Mesoporous Materials. ChemPhysChem, 2010, 11, 1757-1762.	1.0	12
53	â€œHotâ€•Surface Activation of Molecular Complexes: Insight from Modeling Studies. Angewandte Chemie - International Edition, 2010, 49, 1944-1948.	7.2	50
54	Interactions, Behavior, And Stability of Fluorenone inside Zeolite Nanochannels. Journal of Physical Chemistry C, 2010, 114, 10572-10579.	1.5	49

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55	TS-1 from First Principles. Journal of Physical Chemistry A, 2009, 113, 15006-15015.	1.1	51
56	Innovative M(Hfa)2â€¢TMEDA (M=Cu, Co) Precursors for the CVD of Copper-Cobalt Oxides: an Integrated Theoretical and Experimental Approach. ECS Transactions, 2009, 25, 549-556.	0.3	10
57	<scp>l</scp>â€Lactate dehydrogenation in flavocytochrome b₂. FEBS Journal, 2009, 276, 2368-2380.	2.2	18
58	Vaporâ€“liquid phase equilibria of water modelled by a Kimâ€“Gordon potential. Chemical Physics Letters, 2009, 479, 60-64.	1.2	2
59	An integrated experimental and theoretical investigation on Cu(hfa)2Â·TMEDA: structure, bonding and reactivity. Physical Chemistry Chemical Physics, 2009, 11, 5998.	1.3	43
60	Bathochromic Effects in Electronic Excitation Spectra of Hydrated Ti Zeolites: A Theoretical Characterization. ChemPhysChem, 2008, 9, 538-543.	1.0	15
61	High pressure deformation mechanism of Li-ABW: Synchrotron XRPD study and ab initio molecular dynamics simulations. Microporous and Mesoporous Materials, 2008, 115, 267-280.	2.2	32
62	Influence of silanols condensation on surface properties of micelle-templated silicas: A modelling study. Microporous and Mesoporous Materials, 2008, 116, 718-722.	2.2	11
63	Water in Acid Boralites: Hydration Effects on Framework B Sites. Journal of Physical Chemistry C, 2008, 112, 15394-15401.	1.5	16
64	First principles studies on boron sites. Studies in Surface Science and Catalysis, 2008, 174, 751-754.	1.5	3
65	Understanding the Vibrational and Electronic Features of Ti(IV) Sites in Mesoporous Silicas by Integrated Ab Initio and Spectroscopic Investigations. Journal of Physical Chemistry C, 2007, 111, 4946-4955.	1.5	37
66	First Principles Studies on Boron Sites in Zeolites. Journal of Physical Chemistry A, 2007, 111, 11626-11637.	1.1	24
67	Does Negative Hyperconjugation Assist Enzymatic Dehydrogenations?. ChemPhysChem, 2007, 8, 1283-1288.	1.0	8
68	Gismondine under HP: Deformation mechanism and re-organization of the extra-framework species. Microporous and Mesoporous Materials, 2007, 103, 190-209.	2.2	40
69	Properties of defect centres on nanothick silica layers: an abÂinitio investigation. Journal of Porous Materials, 2007, 14, 339-347.	1.3	4
70	On the Role of Ti(IV) as a Lewis Acid in the Chemistry of Titanium Zeolites:Â Formation, Structure, Reactivity, and Aging of Tiâ^'Peroxo Oxidizing Intermediates. A First Principles Study. Journal of Physical Chemistry B, 2006, 110, 21651-21661.	1.2	47
71	Intermolecular Electronic Excitation Transfer in a Confined Space: A First-Principles Study. ChemPhysChem, 2005, 6, 1917-1922.	1.0	12
72	Electronic Spectra of Ti(IV) in Zeolites: An Ab Initio Approach. ChemPhysChem, 2005, 6, 1237-1239.	1.0	19

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73	The â€œtemplateâ€•effect of the extra-framework content on zeolite compression: The case of yugawaralite. American Mineralogist, 2005, 90, 28-35.	0.9	41
74	A density-functional approach to polarizable models: A Kim-Gordon response density interaction potential for molecular simulations. Journal of Chemical Physics, 2005, 123, 074108.	1.2	14
75	Dehydration dynamics of bikitaite: Part II. Ab initio molecular dynamics study. American Mineralogist, 2004, 89, 102-109.	0.9	33
76	Rotation of molecules and ions in confined spaces: a first-principles simulation study. Journal of Molecular Structure, 2003, 644, 55-66.	1.8	11
77	Ab Initio Study of Defect Sites at the Inner Surfaces of Mesoporous Silicas. Journal of Physical Chemistry B, 2003, 107, 10767-10772.	1.2	36
78	Structural deformation mechanisms of zeolites under pressure. American Mineralogist, 2003, 88, 1416-1422.	0.9	60
79	High-pressure behavior of bikitaite: An integrated theoretical and experimental approach. American Mineralogist, 2002, 87, 1415-1425.	0.9	56
80	First-Principles Study of Aqueous Hydroxide Solutions. Journal of the American Chemical Society, 2002, 124, 8534-8535.	6.6	86
81	Classical polarizable force fields parametrized from ab initio calculations. Journal of Chemical Physics, 2002, 117, 1416-1433.	1.2	61
82	Water Molecules in Single File:Â First-Principles Studies of One-Dimensional Water Chains in Zeolites. Journal of Physical Chemistry B, 2001, 105, 3012-3016.	1.2	48
83	On the collective properties of water molecules in one-dimensional zeolitic channels. Physical Chemistry Chemical Physics, 2001, 3, 4158-4163.	1.3	51
84	Intracage chemistry: nitrite to nitrate oxidation via molecular oxygen. A Car Parrinello study.. Studies in Surface Science and Catalysis, 2001, 140, 251-268.	1.5	3
85	First-principles simulation of the intracage oxidation of nitrite to nitrate sodalite. Chemical Physics Letters, 2000, 329, 1-6.	1.2	13
86	Dipolar host/guest interactions and geometrical confinement at the basis of the stability of one-dimensional ice in zeolite bikitaite. Journal of Chemical Physics, 1999, 111, 355-359.	1.2	38
87	One-dimensional ice in bikitaite: single-crystal X-ray diffraction, infra-red spectroscopy and ab-initio molecular dynamics studies. Microporous and Mesoporous Materials, 1999, 30, 77-87.	2.2	40
88	Ab initio molecular dynamics study of the Brnsted acid site in a gallium zeolite. Physical Chemistry Chemical Physics, 1999, 1, 531-536.	1.3	17
89	Study of electrostatic properties in three model sodalites: A different perspective on brÃ¸nsted acidity and host-guest interactions in zeolitic cages. Studies in Surface Science and Catalysis, 1999, 125, 285-292.	1.5	6
90	Structure and Dynamics of a BrÃ¸nsted Acid Site in a Zeolite:Â An ab Initio Study of Hydrogen Sodalite. Journal of Physical Chemistry B, 1998, 102, 3974-3979.	1.2	34

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91	A LCAO-LDF study of Brâˆ…nsted acids chemisorption on ZnO(0001). Surface Science, 1996, 352-354, 341-345.	0.8	9
92	An experimental and theoretical study of the interaction of CH3OH and CH3SH with ZnO. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 3247.	1.7	23