

Gloria Tabacchi

List of Publications by Year in descending order

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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	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. <i>Journal of Chemical Physics</i> , 2020, 152, 194103.	1.2	1,371
2	First-Principles Study of Aqueous Hydroxide Solutions. <i>Journal of the American Chemical Society</i> , 2002, 124, 8534-8535.	6.6	86
3	Shape-controlled TiO ₂ nanoparticles and TiO ₂ P25 interacting with CO and H ₂ O ₂ molecular probes: a synergic approach for surface structure recognition and physico-chemical understanding. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 307-315.	1.3	65
4	Î ² -Fe ₂ O ₃ nanomaterials from an iron(II) diketonate-diamine complex: a study from molecular precursor to growth process. <i>Dalton Transactions</i> , 2012, 41, 149-155.	1.6	63
5	Classical polarizable force fields parametrized from ab initio calculations. <i>Journal of Chemical Physics</i> , 2002, 117, 1416-1433.	1.2	61
6	Structural deformation mechanisms of zeolites under pressure. <i>American Mineralogist</i> , 2003, 88, 1416-1422.	0.9	60
7	Supramolecular Organization in Confined Nanospaces. <i>ChemPhysChem</i> , 2018, 19, 1249-1297.	1.0	60
8	The Case of Formic Acid on Anatase TiO ₂ (101): Where is the Acid Proton?. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 12431-12434.	7.2	59
9	High-pressure behavior of bikitaite: An integrated theoretical and experimental approach. <i>American Mineralogist</i> , 2002, 87, 1415-1425.	0.9	56
10	On the collective properties of water molecules in one-dimensional zeolitic channels. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 4158-4163.	1.3	51
11	TS-1 from First Principles. <i>Journal of Physical Chemistry A</i> , 2009, 113, 15006-15015.	1.1	51
12	Surface Activation of Molecular Complexes: Insight from Modeling Studies. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1944-1948.	7.2	50
13	Interactions, Behavior, And Stability of Fluorenone inside Zeolite Nanochannels. <i>Journal of Physical Chemistry C</i> , 2010, 114, 10572-10579.	1.5	49
14	Water Molecules in Single File: First-Principles Studies of One-Dimensional Water Chains in Zeolites. <i>Journal of Physical Chemistry B</i> , 2001, 105, 3012-3016.	1.2	48
15	On the Role of Ti(IV) as a Lewis Acid in the Chemistry of Titanium Zeolites: Formation, Structure, Reactivity, and Aging of Ti ^{IV} Peroxo Oxidizing Intermediates. A First Principles Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21651-21661.	1.2	47
16	Orientation and Order of Xanthene Dyes in the One-Dimensional Channels of Zeolite L: Bridging the Gap between Experimental Data and Molecular Behavior. <i>Journal of Physical Chemistry C</i> , 2012, 116, 16784-16799.	1.5	44
17	Host-Guest Interactions and Orientation of Dyes in the One-Dimensional Channels of Zeolite L. <i>Langmuir</i> , 2013, 29, 9188-9198.	1.6	44
18	The effect of pressure on open-framework silicates: elastic behaviour and crystal-fluid interaction. <i>Physics and Chemistry of Minerals</i> , 2018, 45, 115-138.	0.3	44

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19	An integrated experimental and theoretical investigation on Cu(hfa) ₂ ·TMEDA: structure, bonding and reactivity. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 5998.	1.3	43
20	The "template" effect of the extra-framework content on zeolite compression: The case of yugawaralite. <i>American Mineralogist</i> , 2005, 90, 28-35.	0.9	41
21	Close-Packed Dye Molecules in Zeolite Channels Self-Assemble into Supramolecular Nanoladders. <i>Journal of Physical Chemistry C</i> , 2014, 118, 15732-15743.	1.5	41
22	One-dimensional ice in bikitaite: single-crystal X-ray diffraction, infra-red spectroscopy and ab-initio molecular dynamics studies. <i>Microporous and Mesoporous Materials</i> , 1999, 30, 77-87.	2.2	40
23	Gismondine under HP: Deformation mechanism and re-organization of the extra-framework species. <i>Microporous and Mesoporous Materials</i> , 2007, 103, 190-209.	2.2	40
24	An iron(II) diamine diketonate molecular complex: Synthesis, characterization and application in the CVD of Fe ₂ O ₃ thin films. <i>Inorganica Chimica Acta</i> , 2012, 380, 161-166.	1.2	40
25	Dipolar host/guest interactions and geometrical confinement at the basis of the stability of one-dimensional ice in zeolite bikitaite. <i>Journal of Chemical Physics</i> , 1999, 111, 355-359.	1.2	38
26	First-principles simulation of the absorption bands of fluorenone in zeolite L. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 159-167.	1.3	38
27	Structure of Nanochannel Entrances in Stopcock-Functionalized Zeolite...L Composites. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11112-11116.	7.2	38
28	Understanding the Vibrational and Electronic Features of Ti(IV) Sites in Mesoporous Silicas by Integrated Ab Initio and Spectroscopic Investigations. <i>Journal of Physical Chemistry C</i> , 2007, 111, 4946-4955.	1.5	37
29	Ab Initio Study of Defect Sites at the Inner Surfaces of Mesoporous Silicas. <i>Journal of Physical Chemistry B</i> , 2003, 107, 10767-10772.	1.2	36
30	Structure and Dynamics of a Brønsted Acid Site in a Zeolite: An ab Initio Study of Hydrogen Sodalite. <i>Journal of Physical Chemistry B</i> , 1998, 102, 3974-3979.	1.2	34
31	Manganese(II) Molecular Sources for Plasma-Assisted CVD of Mn Oxides and Fluorides: From Precursors to Growth Process. <i>Journal of Physical Chemistry C</i> , 2018, 122, 1367-1375.	1.5	34
32	Dehydration dynamics of bikitaite: Part II. Ab initio molecular dynamics study. <i>American Mineralogist</i> , 2004, 89, 102-109.	0.9	33
33	One-dimensional self-assembly of perylene-diimide dyes by unidirectional transit of zeolite channel openings. <i>Chemical Communications</i> , 2016, 52, 11195-11198.	2.2	33
34	Irreversible Conversion of a Water-Ethanol Solution into an Organized Two-Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 2105-2109.	7.2	33
35	Molecular Engineering of Mn ^{II} Diamine Diketone Precursors for the Vapor Deposition of Manganese Oxide Nanostructures. <i>Chemistry - A European Journal</i> , 2017, 23, 17954-17963.	1.7	33
36	High pressure deformation mechanism of Li-ABW: Synchrotron XRPD study and ab initio molecular dynamics simulations. <i>Microporous and Mesoporous Materials</i> , 2008, 115, 267-280.	2.2	32

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37	Precision Molecular Threading/Dethreading. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14825-14834.	7.2	32
38	How Does Cu ^{II} Convert into Cu ^I ? An Unexpected Ring-Mediated Single-Electron Reduction. <i>Chemistry - A European Journal</i> , 2011, 17, 10864-10870.	1.7	31
39	Surface features of TiO ₂ nanoparticles: combination modes of adsorbed CO probe the stepping of (101) facets. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13391.	1.3	28
40	On the Simple Complexity of Carbon Monoxide on Oxide Surfaces: Facet-Specific Donation and Backdonation Effects Revealed on TiO ₂ Anatase Nanoparticles. <i>ChemPhysChem</i> , 2016, 17, 1956-1960.	1.0	28
41	Sensing Nitrogen Mustard Gas Simulant at the ppb Scale via Selective Dual-Site Activation at Au/Mn ₃ O ₄ Interfaces. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23692-23700.	4.0	26
42	First Principles Studies on Boron Sites in Zeolites. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11626-11637.	1.1	24
43	CVD precursors for transition metal oxide nanostructures: molecular properties, surface behavior and temperature effects. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2014, 211, 251-259.	0.8	24
44	An experimental and theoretical study of the interaction of CH ₃ OH and CH ₃ SH with ZnO. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996, 92, 3247.	1.7	23
45	Structure and Host-Guest Interactions of Perylene-Diimide Dyes in Zeolite L Nanochannels. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3401-3418.	1.5	22
46	Opening the Pandora's jar of molecule-to-material conversion in chemical vapor deposition: Insights from theory. <i>International Journal of Quantum Chemistry</i> , 2014, 114, 1-7.	1.0	20
47	Electronic Spectra of Ti(IV) in Zeolites: An Ab Initio Approach. <i>ChemPhysChem</i> , 2005, 6, 1237-1239.	1.0	19
48	Lactate dehydrogenation in flavocytochrome <i>b₂</i> . <i>FEBS Journal</i> , 2009, 276, 2368-2380.	2.2	18
49	Engineering Au/MnO ₂ hierarchical nanoarchitectures for ethanol electrochemical valorization. <i>Journal of Materials Chemistry A</i> , 2020, 8, 16902-16907.	5.2	18
50	Ab initio molecular dynamics study of the Brønsted acid site in a gallium zeolite. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 531-536.	1.3	17
51	Dethreading of a Photoactive Azobenzene-Containing Molecular Axle from a Crown Ether Ring: A Computational Investigation. <i>ChemPhysChem</i> , 2016, 17, 1913-1919.	1.0	17
52	Water in Acid Borates: Hydration Effects on Framework B Sites. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15394-15401.	1.5	16
53	Bathochromic Effects in Electronic Excitation Spectra of Hydrated Ti Zeolites: A Theoretical Characterization. <i>ChemPhysChem</i> , 2008, 9, 538-543.	1.0	15
54	Unravelling the High-Pressure Behaviour of Dye-Zeolite L Hybrid Materials. <i>Crystals</i> , 2018, 8, 79.	1.0	15

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55	Differential penetration of ethanol and water in Si-chabazite: High pressure dehydration of azeotrope solution. <i>Microporous and Mesoporous Materials</i> , 2019, 284, 161-169.	2.2	15
56	Chemically Induced Mismatch of Rings and Stations in [3]Rotaxanes. <i>Journal of the American Chemical Society</i> , 2021, 143, 8046-8055.	6.6	15
57	A density-functional approach to polarizable models: A Kim-Gordon response density interaction potential for molecular simulations. <i>Journal of Chemical Physics</i> , 2005, 123, 074108.	1.2	14
58	First-principles simulation of the intracage oxidation of nitrite to nitrate sodalite. <i>Chemical Physics Letters</i> , 2000, 329, 1-6.	1.2	13
59	Intermolecular Electronic Excitation Transfer in a Confined Space: A First-Principles Study. <i>ChemPhysChem</i> , 2005, 6, 1917-1922.	1.0	12
60	On the Compatibility Criteria for Protein Encapsulation inside Mesoporous Materials. <i>ChemPhysChem</i> , 2010, 11, 1757-1762.	1.0	12
61	Behaviour at high pressure of Rb ₇ NaGa ₈ Si ₁₂ O ₄₀ ·3H ₂ O (a zeolite with EDI topology): a combined experimental-computational study. <i>Physics and Chemistry of Minerals</i> , 2016, 43, 209-216.	0.3	12
62	Rotation of molecules and ions in confined spaces: a first-principles simulation study. <i>Journal of Molecular Structure</i> , 2003, 644, 55-66.	1.8	11
63	Influence of silanols condensation on surface properties of micelle-templated silicas: A modelling study. <i>Microporous and Mesoporous Materials</i> , 2008, 116, 718-722.	2.2	11
64	Disentangling protein-silica interactions. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 1463-1477.	1.6	11
65	Innovative M(Hfa) ₂ TMEDA (M=Cu, Co) Precursors for the CVD of Copper-Cobalt Oxides: an Integrated Theoretical and Experimental Approach. <i>ECS Transactions</i> , 2009, 25, 549-556.	0.3	10
66	The Case of Formic Acid on Anatase TiO ₂ (101): Where is the Acid Proton?. <i>Angewandte Chemie</i> , 2019, 131, 12561-12564.	1.6	10
67	Water in zeolite L and its MOF mimic. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2019, 234, 495-511.	0.4	10
68	Precision Molecular Threading/Dethreading. <i>Angewandte Chemie</i> , 2020, 132, 14935-14944.	1.6	10
69	A LCAO-LDF study of Brønsted acids chemisorption on ZnO(0001). <i>Surface Science</i> , 1996, 352-354, 341-345.	0.8	9
70	Facile preparation of a cobalt diamine diketonate adduct as a potential vapor phase precursor for Co ₃ O ₄ films. <i>Dalton Transactions</i> , 2021, 50, 10374-10385.	1.6	9
71	The Early Steps of Molecule-to-Material Conversion in Chemical Vapor Deposition (CVD): A Case Study. <i>Molecules</i> , 2021, 26, 1988.	1.7	9
72	Does Negative Hyperconjugation Assist Enzymatic Dehydrogenations?. <i>ChemPhysChem</i> , 2007, 8, 1283-1288.	1.0	8

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73	Computer modeling of apparently straight bond angles: The intriguing case of all-silica ferrierite. <i>American Mineralogist</i> , 2019, 104, 1546-1555.	0.9	8
74	Pressure-Induced Penetration of Water-Ethanol Mixtures in All-Silica Ferrierite. <i>Advanced Science Letters</i> , 2017, 23, 5966-5969.	0.2	8
75	Confining a Protein-Containing Water Nanodroplet inside Silica Nanochannels. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2965.	1.8	7
76	Steering polymer growth by molding nanochannels: 1,5-hexadiene polymerization in high silica mordenite. <i>Microporous and Mesoporous Materials</i> , 2021, 311, 110728.	2.2	7
77	A versatile Fe(II) diketonate diamine adduct: Preparation, characterization and validation in the chemical vapor deposition of iron oxide nanomaterials. <i>Materials Chemistry and Physics</i> , 2022, 277, 125534.	2.0	7
78	Study of electrostatic properties in three model sodalites: A different perspective on brønsted acidity and host-guest interactions in zeolitic cages. <i>Studies in Surface Science and Catalysis</i> , 1999, 125, 285-292.	1.5	6
79	Irreversible Conversion of a Water-Ethanol Solution into an Organized Two-Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure. <i>Angewandte Chemie</i> , 2017, 129, 2137-2141.	1.6	6
80	Does the Abiotic Formation of Oligopeptides on TiO ₂ Nanoparticles Require Special Catalytic Sites? Apparently Not. <i>Journal of Nanoscience and Nanotechnology</i> , 2018, 18, 5854-5857.	0.9	5
81	Properties of defect centres on nanothick silica layers: an ab initio investigation. <i>Journal of Porous Materials</i> , 2007, 14, 339-347.	1.3	4
82	High-silica mordenite as scaffold for phenylacetylene polymerization: In situ high pressure investigation. <i>Microporous and Mesoporous Materials</i> , 2020, 300, 110163.	2.2	4
83	Intracage chemistry: nitrite to nitrate oxidation via molecular oxygen. A Car Parrinello study.. <i>Studies in Surface Science and Catalysis</i> , 2001, 140, 251-268.	1.5	3
84	First principles studies on boron sites. <i>Studies in Surface Science and Catalysis</i> , 2008, 174, 751-754.	1.5	3
85	A post-HF approach to the sunscreen octyl methoxycinnamate. <i>Journal of Chemical Physics</i> , 2021, 154, 144304.	1.2	3
86	Spontaneous polymerization of benzofulvene derivatives bearing complexed or un-complexed pyridine rings. <i>European Polymer Journal</i> , 2022, 169, 111137.	2.6	3
87	Vapor-liquid phase equilibria of water modelled by a Kim-Gordon potential. <i>Chemical Physics Letters</i> , 2009, 479, 60-64.	1.2	2
88	Titelbild: The Case of Formic Acid on Anatase TiO ₂ (101): Where is the Acid Proton? (Angew.) <i>Tj ETQq 0,0 0 rgBT /Overlock I</i>	1.6	1
89	Effective transport of electronic excitation energy through zeolite channels: a structural study. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2015, 71, s300-s300.	0.0	0
90	Structural modification of gallium lanthanum sulfide glass induced by ultrafast laser inscription. , 2017, , .		0

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91	Titelbild: Irreversible Conversion of a Water/Ethanol Solution into an Organized Two-Dimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure (Angew. Chem.) Tj ETQq1 1 0.784314 0gBT /Over	0.0	0
92	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