Ettore S Fois

List of Publications by Year
in descending order

121 papers	3,139 citations	126708 33 h-index	197535 49 g-index
131 all docs	131 docs citations	131 times ranked	2486 citing authors

#	Article	IF	Citations
1	Molecular dynamics studies on zeolites. 4. Diffusion of methane in silicalite. The Journal of Physical Chemistry, 1990, 94, 4329-4334.	2.9	168
2	Surface Structure of TiO₂ P25 Nanoparticles: Infrared Study of Hydroxy Groups on Coordinative Defect Sites. Journal of Physical Chemistry C, 2010, 114, 21531-21538.	1.5	164
3	Properties of supercritical water: an ab initio simulation. Chemical Physics Letters, 1994, 223, 411-415.	1.2	142
4	On the unusual stability of Maya blue paint: molecular dynamics simulations. Microporous and Mesoporous Materials, 2003, 57, 263-272.	2.2	107
5	The Color and Stability of Maya Blue: TDDFT Calculations. Journal of Physical Chemistry C, 2009, 113, 8683-8687.	1.5	78
6	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
7	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
8	Molecular dynamics studies on zeolites. II: A simple model for silicates applied to anhydrous natrolite. Zeolites, 1987, 7, 522-527.	0.9	61
9	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
10	High-pressure behavior of bikitaite: An integrated theoretical and experimental approach. American Mineralogist, 2002, 87, 1415-1425.	0.9	56
11	Approach to metallic behavior in metalâ€“molten-salt solutions. Physical Review B, 1989, 39, 4812-4815.	1.1	53
12	On the collective properties of water molecules in one-dimensional zeolitic channels. Physical Chemistry Chemical Physics, 2001, 3, 4158-4163.	1.3	51
13	TS-1 from First Principles. Journal of Physical Chemistry A, 2009, 113, 15006-15015.	1.1	51
14	â€œHotâ€•Surface Activation of Molecular Complexes: Insight from Modeling Studies. Angewandte Chemie - International Edition, 2010, 49, 1944-1948.	7.2	50
15	Interactions, Behavior, And Stability of Fluorenone inside Zeolite Nanochannels. Journal of Physical Chemistry C, 2010, 114, 10572-10579.	1.5	49
16	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
17	Structure, electronic properties, and defects of amorphous gallium arsenide. Physical Review B, 1992, 45, 13378-13382.	1.1	47
18	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

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19	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
20	Hostâ€“Guest Interactions and Orientation of Dyes in the One-Dimensional Channels of Zeolite L. Langmuir, 2013, 29, 9188-9198.	1.6	44
21	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
22	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
23	Close-Packed Dye Molecules in Zeolite Channels Self-Assemble into Supramolecular Nanoladders. Journal of Physical Chemistry C, 2014, 118, 15732-15743.	1.5	41
24	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
25	Structure and Dynamics of the Flexible Triple Helix of Water inside VPI-5 Molecular Sieves. Journal of Physical Chemistry B, 2002, 106, 4806-4812.	1.2	40
26	Gismondine under HP: Deformation mechanism and re-organization of the extra-framework species. Microporous and Mesoporous Materials, 2007, 103, 190-209.	2.2	40
27	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
28	First-principles simulation of the absorption bands of fluorenone in zeolite L. Physical Chemistry Chemical Physics, 2013, 15, 159-167.	1.3	38
29	Structure of Nanochannel Entrances in Stopcockâ€Functionalized Zeoliteâ€…L Composites. Angewandte Chemie - International Edition, 2015, 54, 11112-11116.	7.2	38
30	Molecular dynamics studies on zeolites. Part 5.â€”Discussion of the structural changes of silicalite. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1657-1663.	1.7	37
31	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
32	Selfâ€interaction corrected density functionals and the structure of metal clusters. Journal of Chemical Physics, 1993, 98, 6352-6360.	1.2	36
33	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
34	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
35	Dehydration dynamics of bikitaite: Part II. Ab initio molecular dynamics study. American Mineralogist, 2004, 89, 102-109.	0.9	33
36	One-dimensional self-assembly of perylene-diimide dyes by unidirectional transit of zeolite channel openings. Chemical Communications, 2016, 52, 11195-11198.	2.2	33

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37	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
38	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
39	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
40	Precision Molecular Threading/Dethreading. Angewandte Chemie - International Edition, 2020, 59, 14825-14834.	7.2	32
41	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
42	First-Principles Molecular Dynamics Investigation of thed-Amino Acid Oxidative Half-Reaction Catalyzed by the Flavoenzymed-Amino Acid Oxidaseâ€,â€¡. Biochemistry, 2002, 41, 14111-14121.	1.2	28
43	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
44	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
45	Hydrophobic effects: A computer simulation study of the temperature influence in dilute O2 aqueous solutions. Journal of Chemical Physics, 1999, 110, 1025-1035.	1.2	27
46	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
47	Control of the adiabatic electronic state in ab initio molecular dynamics. Journal of Chemical Physics, 1993, 98, 6361-6368.	1.2	25
48	Ab Initio Molecular Dynamics Simulation of the Interaction between Water and Ti in Zeolitic Systems. Journal of Physical Chemistry B, 2004, 108, 154-159.	1.2	25
49	Static and dynamic density functional investigation of hydrated beryllium dications. International Journal of Quantum Chemistry, 1996, 57, 655-662.	1.0	24
50	Dehydration dynamics of bikitaite: Part I. In situ synchrotron powder X-ray diffraction study. American Mineralogist, 2004, 89, 94-101.	0.9	24
51	First Principles Studies on Boron Sites in Zeolites. Journal of Physical Chemistry A, 2007, 111, 11626-11637.	1.1	24
52	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
53	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
54	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

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55	Electronic Spectra of Ti(IV) in Zeolites: An Ab Initio Approach. ChemPhysChem, 2005, 6, 1237-1239.	1.0	19
56	<scp>l</scp>â€Lactate dehydrogenation in flavocytochrome b₂. FEBS Journal, 2009, 276, 2368-2380.	2.2	18
57	Engineering Au/MnO₂ hierarchical nanoarchitectures for ethanol electrochemical valorization. Journal of Materials Chemistry A, 2020, 8, 16902-16907.	5.2	18
58	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
59	Competition between Water and Hydrogen Peroxide at Ti Center in Titanium Zeolites. An ab Initio Study. Journal of Physical Chemistry B, 2004, 108, 9557-9560.	1.2	17
60	Dethreading of a Photoactive Azobenzeneâ€Containing Molecular Axle from a Crown Ether Ring: A Computational Investigation. ChemPhysChem, 2016, 17, 1913-1919.	1.0	17
61	Ab initio and semiempirical study of the energy and geometry of ion-molecule pairs. 5. Vinyldiazonium cation in vacuo and in solution. The Journal of Physical Chemistry, 1982, 86, 3722-3728.	2.9	16
62	A potential for molecular dynamics simulations of structural and dynamic properties of hydrate aluminosilicates. Materials Chemistry and Physics, 1991, 29, 357-367.	2.0	16
63	A molecular dynamics study of the behavior of sodium in low albite. American Mineralogist, 2003, 88, 1-10.	0.9	16
64	Water in Acid Boralites: Hydration Effects on Framework B Sites. Journal of Physical Chemistry C, 2008, 112, 15394-15401.	1.5	16
65	An implemented potential of non-rigid water molecules for molecular dynamics simulations. Chemical Physics Letters, 1986, 127, 456-461.	1.2	15
66	Bathochromic Effects in Electronic Excitation Spectra of Hydrated Ti Zeolites: A Theoretical Characterization. ChemPhysChem, 2008, 9, 538-543.	1.0	15
67	Unravelling the High-Pressure Behaviour of Dye-Zeolite L Hybrid Materials. Crystals, 2018, 8, 79.	1.0	15
68	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
69	Chemically Induced Mismatch of Rings and Stations in [3]Rotaxanes. Journal of the American Chemical Society, 2021, 143, 8046-8055.	6.6	15
70	A theoretical investigation of energetics and structures of CH5+(CH4)n clusters for nâ€,=â€,1â€“4. Canadian Journal of Chemistry, 1985, 63, 1468-1472.	0.6	14
71	First-principles simulation of the intracage oxidation of nitrite to nitrate sodalite. Chemical Physics Letters, 2000, 329, 1-6.	1.2	13
72	Host/Guest Interactions and Femtosecond Scale Proton Exchange in a Zeolitic Cage. Journal of Physical Chemistry B, 1997, 101, 4487-4489.	1.2	12

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73	Intermolecular Electronic Excitation Transfer in a Confined Space: A First-Principles Study. ChemPhysChem, 2005, 6, 1917-1922.	1.0	12
74	On the Compatibility Criteria for Protein Encapsulation inside Mesoporous Materials. ChemPhysChem, 2010, 11, 1757-1762.	1.0	12
75	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
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	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
78	Disentangling proteinâ€“silica interactions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1463-1477.	1.6	11
79	Theoretical study of the solvation of nitrogen. Two different approaches. Theoretica Chimica Acta, 1981, 58, 97-109.	0.9	10
80	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
81	The Case of Formic Acid on Anatase TiO 2 (101): Where is the Acid Proton?. Angewandte Chemie, 2019, 131, 12561-12564.	1.6	10
82	Water in zeolite L and its MOF mimic. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 495-511.	0.4	10
83	Precision Molecular Threading/Dethreading. Angewandte Chemie, 2020, 132, 14935-14944.	1.6	10
84	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
85	The Early Steps of Molecule-to-Material Conversion in Chemical Vapor Deposition (CVD): A Case Study. Molecules, 2021, 26, 1988.	1.7	9
86	Monte Carlo studies of aqueous solution of nitrogen using different potential energy surfaces. Molecular Physics, 1986, 58, 65-83.	0.8	8
87	Dynamical Host/Guest Interactions in Zeolites:Â Framework Isotope Effects on Proton Transfer Studied by Carâ^'Parrinello Molecular Dynamics. Journal of Physical Chemistry B, 1999, 103, 1794-1799.	1.2	8
88	The role of extra-framework cations on the structure of dehydrated Li-ABW. A computer simulation study. Microporous and Mesoporous Materials, 2003, 57, 73-81.	2.2	8
89	Does Negative Hyperconjugation Assist Enzymatic Dehydrogenations?. ChemPhysChem, 2007, 8, 1283-1288.	1.0	8
90	Computer modeling of apparently straight bond angles: The intriguing case of all-silica ferrierite. American Mineralogist, 2019, 104, 1546-1555.	0.9	8

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91	Pressure-Induced Penetration of Water-Ethanol Mixtures in All-Silica Ferrierite. Advanced Science Letters, 2017, 23, 5966-5969.	0.2	8
92	A theoretical investigation of the role of the solvent on the structure of the intermediates in solvolytic reactions. Part 4. Methanediazonium ion and methyl fluoride in hydrofluoric acid. Journal of the Chemical Society Perkin Transactions II, 1982, , 783.	0.9	7
93	Structure and dynamics of nitrite sodalite. Anab initio study. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 1679-1685.	0.4	7
94	Confining a Protein-Containing Water Nanodroplet inside Silica Nanochannels. International Journal of Molecular Sciences, 2019, 20, 2965.	1.8	7
95	Steering polymer growth by molding nanochannels: 1,5-hexadiene polymerization in high silica mordenite. Microporous and Mesoporous Materials, 2021, 311, 110728.	2.2	7
96	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
97	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
98	Irreversible Conversion of a Waterâ€“Ethanol Solution into an Organized Twoâ€Ðimensional Network of Alternating Supramolecular Units in a Hydrophobic Zeolite under Pressure. Angewandte Chemie, 2017, 129, 2137-2141.	1.6	6
99	Polarized emission and mechanofluorochromism of benzothiadiazole based chromophores oriented by rubbing. Dyes and Pigments, 2022, 204, 110473.	2.0	6
100	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
101	A method for correcting empirical potentials. Application to water molecule.. Computational and Theoretical Chemistry, 1985, 120, 201-206.	1.5	4
102	Electronic properties of new zeolitic supra-lattices. Physical Chemistry Chemical Physics, 2001, 3, 1877-1882.	1.3	4
103	Properties of defect centres on nanothick silica layers: an abÂinitio investigation. Journal of Porous Materials, 2007, 14, 339-347.	1.3	4
104	UV-light-induced polymerization in the amorphous solid-state of a spontaneously non-polymerizing 3-phenylbenzofulvene monomer. European Polymer Journal, 2020, 137, 109923.	2.6	4
105	High-silica mordenite as scaffold for phenylacetylene polymerization: In situ high pressure investigation. Microporous and Mesoporous Materials, 2020, 300, 110163.	2.2	4
106	Monte Carlo calculations on structural and thermodynamic characteristics for acetone and the Na+-acetone system at 298 K. Journal of Structural Chemistry, 1989, 30, 267-272.	0.3	3
107	A density functional study of the aluminium dimer. Computational and Theoretical Chemistry, 1992, 261, 277-285.	1.5	3
108	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

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109	First principles studies on boron sites. Studies in Surface Science and Catalysis, 2008, 174, 751-754.	1.5	3
110	Solvent-free synthesis of Serâ€“His dipeptide from non-activated amino acids and its potential function as organocatalyst. Research on Chemical Intermediates, 2018, 44, 1797-1810.	1.3	3
111	A post-HF approach to the sunscreen octyl methoxycinnamate. Journal of Chemical Physics, 2021, 154, 144304.	1.2	3
112	Synthesis and UV-light induced oligomerization of a benzofulvene-based neutral platinum(II) complex. European Polymer Journal, 2021, 156, 110597.	2.6	3
113	Spontaneous polymerization of benzofulvene derivatives bearing complexed or un-complexed pyridine rings. European Polymer Journal, 2022, 169, 111137.	2.6	3
114	Solvated alkali atoms and electronâ€transfer paramagnetic ion pairs: Some common trends from computer simulation studies. Journal of Chemical Physics, 1994, 100, 9044-9049.	1.2	2
115	On the adiabatic dynamics of paramagnetic ion pairs. Applied Magnetic Resonance, 1992, 3, 841-848.	0.6	1
116	Charge layering in polar liquids. Chemical Physics Letters, 1992, 200, 333-336.	1.2	1
117	Titelbild: The Case of Formic Acid on Anatase TiO₂(101): Where is the Acid Proton? (Angew.) Tj ETQq1 1 0.784314 rgBT	1.6	1
118	Ab Initio Molecular Dynamics Applied to Molecular Systems. AIP Conference Proceedings, 1991, , .	0.3	0
119	Competition Between Water and Hydrogen Peroxide at Ti Center in Titanium Zeolites. An ab initio Study.. ChemInform, 2004, 35, no.	0.1	0
120	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
121	Selected Peer-Reviewed Articles from the VI Workshop on Oxide-Based Materials â€œPerspectives in Material Science and Technological Applicationsâ€•(OXIDE 2016), Naples, Italy, 21â€“24 September 2016. Advanced Science Letters, 2017, 23, 5819-5820.	0.2	0