Antonio Tilocca

List of Publications by Year
in descending order

72	4,164	81743 39	110170 64
papers	citations	h-index	g-index

72	72	72	3474
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Dynamical descriptors of bioactivity: a correlation between chemical durability and ion migration in biodegradable glasses. Physical Chemistry Chemical Physics, 2017, 19, 6334-6337.	1.3	5
2	Reactive molecular dynamics: an effective tool for modelling the solâ€“gel synthesis of bioglasses. Journal of Materials Science, 2017, 52, 9006-9013.	1.7	25
3	Influence of Calcium on the Initial Stages of the Solâ€“Gel Synthesis of Bioactive Glasses. Journal of Physical Chemistry B, 2016, 120, 11773-11780.	1.2	25
4	The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations. Biomedical Glasses, 2016, 2, .	2.4	9
5	Realistic Models of Bioactive Glass Radioisotope Vectors in Practical Conditions: Structural Effects of Ion Exchange. Journal of Physical Chemistry C, 2015, 119, 27442-27448.	1.5	13
6	Rationalizing the Biodegradation of Glasses for Biomedical Applications Through Classical and Ab-initio Simulations. Springer Series in Materials Science, 2015, , 255-273.	0.4	2
7	Ab initio simulations of the structure of thin water layers on defective anatase <scp>T</scp>i<scp>O</scp>₂(101) surfaces. International Journal of Quantum Chemistry, 2015, 115, 1250-1257.	1.0	20
8	Structure-solubility relationships in fluoride-containing phosphate based bioactive glasses. Journal of Materials Chemistry B, 2015, 3, 9360-9373.	2.9	25
9	Atomic-scale models of early-stage alkali depletion and SiO₂-rich gel formation in bioactive glasses. Physical Chemistry Chemical Physics, 2015, 17, 2696-2702.	1.3	12
10	Role of glass structure in defining the chemical dissolution behavior, bioactivity and antioxidant properties of zinc and strontium co-doped alkali-free phosphosilicate glasses. Acta Biomaterialia, 2014, 10, 3264-3278.	4.1	64
11	Current challenges in atomistic simulations of glasses for biomedical applications. Physical Chemistry Chemical Physics, 2014, 16, 3874-3880.	1.3	23
12	Probing the fate of interstitial water in bulk bioactive glass by ab initio simulations. RSC Advances, 2014, 4, 36425-36436.	1.7	14
13	Toward a Rational Design of Bioactive Glasses with Optimal Structural Features: Compositionâ€“Structure Correlations Unveiled by Solid-State NMR and MD Simulations. Journal of Physical Chemistry B, 2014, 118, 833-844.	1.2	54
14	Structural role of zinc in biodegradation of alkali-free bioactive glasses. Journal of Materials Chemistry B, 2013, 1, 3073.	2.9	54
15	Hydration Effects on the Structural and Vibrational Properties of Yttrium Aluminosilicate Glasses for in Situ Radiotherapy. Journal of Physical Chemistry B, 2013, 117, 14518-14528.	1.2	11
16	Cooling rate and size effects on the medium-range structure of multicomponent oxide glasses simulated by molecular dynamics. Journal of Chemical Physics, 2013, 139, 114501.	1.2	57
17	Structure and biological activity of glasses and ceramics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 1271-1280.	1.6	32
18	Integrating biological activity into radioisotope vectors: molecular dynamics models of yttrium-doped bioactive glasses. Journal of Materials Chemistry, 2012, 22, 12023.	6.7	37

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19	Molecular Dynamics Simulations and Structural Descriptors of Radioisotope Glass Vectors for In Situ Radiotherapy. Journal of Physical Chemistry B, 2012, 116, 12614-12620.	1.2	28
20	DFT-GGA and DFT+U Simulations of Thin Water Layers on Reduced TiO₂ Anatase. Journal of Physical Chemistry C, 2012, 116, 9114-9121.	1.5	56
21	Molecular Dynamics Methods for Modeling Complex Interactions in Biomaterials. Methods in Molecular Biology, 2012, 811, 285-301.	0.4	4
22	Bioactive glasses as potential radioisotope vectors for in situ cancer therapy: investigating the structural effects of yttrium. Physical Chemistry Chemical Physics, 2011, 13, 17749.	1.3	65
23	Molecular dynamics simulations of a bioactive glass nanoparticle. Journal of Materials Chemistry, 2011, 21, 12660.	6.7	28
24	Fluorine Environment in Bioactive Glasses: ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 2038-2045.	1.2	79
25	The initial stages of bioglass dissolution: a Carâ€“Parrinello molecular-dynamics study of the glassâ€“water interface. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 2102-2111.	1.0	39
26	Shortâ€Range Structure of Yttrium Aluminoâ€Silicate Glass for Cancer Radiotherapy: Carâ€“Parrinello Molecular Dynamics Simulations. Advanced Engineering Materials, 2010, 12, B326.	1.6	26
27	Sodium migration pathways in multicomponent silicate glasses: Carâ€“Parrinello molecular dynamics simulations. Journal of Chemical Physics, 2010, 133, 014701.	1.2	70
28	Surface Signatures of Bioactivity: MD Simulations of 45S and 65S Silicate Glasses. Langmuir, 2010, 26, 545-551.	1.6	73
29	Aluminosilicate Glasses As Yttrium Vectors for in situ Radiotherapy: Understanding Composition-Durability Effects through Molecular Dynamics Simulations. Chemistry of Materials, 2010, 22, 3725-3734.	3.2	52
30	Models of structure, dynamics and reactivity of bioglasses: a review. Journal of Materials Chemistry, 2010, 20, 6848.	6.7	89
31	Structural models of bioactive glasses from molecular dynamics simulations. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2009, 465, 1003-1027.	1.0	133
32	Local ordering and electronic signatures of submonolayer water on anatase TiO2(101). Nature Materials, 2009, 8, 585-589.	13.3	298
33	Modeling the Waterâ€“Bioglass Interface by Ab Initio Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2009, 1, 1324-1333.	4.0	96
34	The Color and Stability of Maya Blue: TDDFT Calculations. Journal of Physical Chemistry C, 2009, 113, 8683-8687.	1.5	78
35	Short- and medium-range structure of multicomponent bioactive glasses and melts: An assessment of the performances of shell-model and rigid-ion potentials. Journal of Chemical Physics, 2008, 129, 084504.	1.2	72
36	Exploring the Surface of Bioactive Glasses: Water Adsorption and Reactivity. Journal of Physical Chemistry C, 2008, 112, 11936-11945.	1.5	56

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37	Structure and dynamics of bioactive phosphosilicate glasses and melts fromab initiomolecular dynamics simulations. Physical Review B, 2007, 76, .	1.1	87
38	The Structure of Bioactive Silicate Glasses:Â New Insight from Molecular Dynamics Simulations. Chemistry of Materials, 2007, 19, 95-103.	3.2	162
39	The formation of nanoscale structures in soluble phosphosilicate glasses for biomedical applications: MD simulations. Faraday Discussions, 2007, 136, 45.	1.6	42
40	Structural Effects of Phosphorus Inclusion in Bioactive Silicate Glasses. Journal of Physical Chemistry B, 2007, 111, 14256-14264.	1.2	145
41	Structural and electronic properties of modified sodium and soda-lime silicate glasses by Carâ€“Parrinello molecular dynamics. Journal of Materials Chemistry, 2006, 16, 1950-1955.	6.7	73
42	Ab Initio Molecular Dynamics Study of 45S5 Bioactive Silicate Glass. Journal of Physical Chemistry B, 2006, 110, 25810-25816.	1.2	62
43	Shell-model molecular dynamics calculations of modified silicate glasses. Physical Review B, 2006, 73, .	1.1	154
44	Mixed dissociated/molecular monolayer of water on the TiO2(011)-(2Ã—1) surface. Surface Science, 2005, 591, L267-L272.	0.8	41
45	O2 and Vacancy Diffusion on Rutile(110): Pathways and Electronic Properties. ChemPhysChem, 2005, 6, 1911-1916.	1.0	69
46	O2Interaction and Reactivity on a Model Hydroxylated Rutile(110) Surface. Journal of Physical Chemistry B, 2005, 109, 20963-20967.	1.2	67
47	Adsorption of Water on Reconstructed Rutile TiO2(011)-(2Ã—1):â€‰ TiO Double Bonds and Surface Reactivity. Journal of the American Chemical Society, 2005, 127, 9895-9903.	6.6	111
48	First-principles string molecular dynamics: An efficient approach for finding chemical reaction pathways. Journal of Chemical Physics, 2004, 121, 3359-3367.	1.2	57
49	Vertical and Lateral Order in Adsorbed Water Layers on Anatase TiO2(101). Langmuir, 2004, 20, 8379-8384.	1.6	130
50	Structure and Reactivity of Water Layers on Defect-Free and Defective Anatase TiO2(101) Surfaces. Journal of Physical Chemistry B, 2004, 108, 4743-4751.	1.2	152
51	Methanol Adsorption and Reactivity on Clean and Hydroxylated Anatase(101) Surfaces. Journal of Physical Chemistry B, 2004, 108, 19314-19319.	1.2	103
52	Time-Dependent DFT Study of [Fe(CN)6]4-Sensitization of TiO2Nanoparticles. Journal of the American Chemical Society, 2004, 126, 15024-15025.	6.6	228
53	On the unusual stability of Maya blue paint: molecular dynamics simulations. Microporous and Mesoporous Materials, 2003, 57, 263-272.	2.2	107
54	Reaction pathway and free energy barrier for defect-induced water dissociation on the (101) surface of TiO2-anatase. Journal of Chemical Physics, 2003, 119, 7445-7450.	1.2	136

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55	Detecting Fabric Defects with a Neural Network Using Two Kinds of Optical Patterns. Textile Reseach Journal, 2002, 72, 545-550.	1.1	42
56	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
57	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
58	Statics and Dynamics of Ethane Molecules in AlPO4-5:Â A Molecular Dynamics Simulation Study. Journal of the American Chemical Society, 2001, 123, 5069-5074.	6.6	44
59	Computer simulations of ethane sorbed in an aluminophosphate molecular sieve. Studies in Surface Science and Catalysis, 2001, , 221-227.	1.5	0
60	An effective harmonic potential for aluminophosphate molecular sieves: application to AlPO4-5. Microporous and Mesoporous Materials, 2001, 42, 103-111.	2.2	17
61	Two- and N-step correlated models for the analysis of molecular dynamics trajectories of linear molecules in silicalite. Journal of Chemical Physics, 2000, 113, 7588-7592.	1.2	9
62	Electric-field-dependent empirical potentials for molecules and crystals: A first application to flexible water molecule adsorbed in zeolites. Journal of Chemical Physics, 2000, 112, 8267-8278.	1.2	37
63	Application of the two-step model to the diffusion of linear diatomic and triatomic molecules in silicalite. Physical Chemistry Chemical Physics, 2000, 2, 1455-1463.	1.3	19
64	Molecular dynamics simulation of an activated transfer reaction in zeolites. Journal of Chemical Physics, 1999, 111, 5529-5543.	1.2	11
65	â€œTwo-stepâ€•model of molecular diffusion in silicalite. Journal of Chemical Physics, 1999, 110, 1163-1172.	1.2	40
66	Recombination Reactions and Diffusive Properties of Diatomic Molecules in Two Different Microporous Structures:â€‰ Silicalite and ZK4. Journal of Physical Chemistry B, 1999, 103, 8141-8152.	1.2	8
67	About the influence of lattice vibrations on the diffusion of methane in a cation-free LTA zeolite. Chemical Physics Letters, 1998, 296, 253-258.	1.2	69
68	A classical molecular dynamics study of recombination reactions in a microporous solid. Journal of Chemical Physics, 1998, 109, 2865-2873.	1.2	8
69	Spectroscopic identification and quantitative analysis of binary mixtures using artificial neural networks. Talanta, 1997, 44, 1901-1909.	2.9	2
70	Molecular dynamics studies of chemical processes in zeolites. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 1665-1671.	0.4	3
71	Diffusion and vibrational relaxation of a diatomic molecule in the pore network of a pure silica zeolite: A molecular dynamics study. Journal of Chemical Physics, 1996, 105, 5586-5594.	1.2	36
72	Chapter 4. Molecular Dynamics Simulations of Bioactive Glass Structure and In vitro Reactivity. RSC Smart Materials, 0, , 89-104.	0.1	1