

Antonio Tilocca

List of Publications by Year in descending order

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72
papers

4,164
citations

81743

39
h-index

110170

64
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72
all docs

72
docs citations

72
times ranked

3474
citing authors

#	ARTICLE	IF	CITATIONS
1	Local ordering and electronic signatures of submonolayer water on anatase TiO ₂ (101). <i>Nature Materials</i> , 2009, 8, 585-589.	13.3	298
2	Time-Dependent DFT Study of [Fe(CN) ₆] ⁴⁻ -Sensitization of TiO ₂ Nanoparticles. <i>Journal of the American Chemical Society</i> , 2004, 126, 15024-15025.	6.6	228
3	The Structure of Bioactive Silicate Glasses: A New Insight from Molecular Dynamics Simulations. <i>Chemistry of Materials</i> , 2007, 19, 95-103.	3.2	162
4	Shell-model molecular dynamics calculations of modified silicate glasses. <i>Physical Review B</i> , 2006, 73, .	1.1	154
5	Structure and Reactivity of Water Layers on Defect-Free and Defective Anatase TiO ₂ (101) Surfaces. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4743-4751.	1.2	152
6	Structural Effects of Phosphorus Inclusion in Bioactive Silicate Glasses. <i>Journal of Physical Chemistry B</i> , 2007, 111, 14256-14264.	1.2	145
7	Reaction pathway and free energy barrier for defect-induced water dissociation on the (101) surface of TiO ₂ -anatase. <i>Journal of Chemical Physics</i> , 2003, 119, 7445-7450.	1.2	136
8	Structural models of bioactive glasses from molecular dynamics simulations. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2009, 465, 1003-1027.	1.0	133
9	Vertical and Lateral Order in Adsorbed Water Layers on Anatase TiO ₂ (101). <i>Langmuir</i> , 2004, 20, 8379-8384.	1.6	130
10	Adsorption of Water on Reconstructed Rutile TiO ₂ (011)-(2 \times 1): \approx TiO Double Bonds and Surface Reactivity. <i>Journal of the American Chemical Society</i> , 2005, 127, 9895-9903.	6.6	111
11	On the unusual stability of Maya blue paint: molecular dynamics simulations. <i>Microporous and Mesoporous Materials</i> , 2003, 57, 263-272.	2.2	107
12	Methanol Adsorption and Reactivity on Clean and Hydroxylated Anatase(101) Surfaces. <i>Journal of Physical Chemistry B</i> , 2004, 108, 19314-19319.	1.2	103
13	Modeling the Water ⁺ Bioglass Interface by Ab Initio Molecular Dynamics Simulations. <i>ACS Applied Materials & Interfaces</i> , 2009, 1, 1324-1333.	4.0	96
14	Models of structure, dynamics and reactivity of bioglasses: a review. <i>Journal of Materials Chemistry</i> , 2010, 20, 6848.	6.7	89
15	Structure and dynamics of bioactive phosphosilicate glasses and melts from <i>ab initio</i> molecular dynamics simulations. <i>Physical Review B</i> , 2007, 76, .	1.1	87
16	Fluorine Environment in Bioactive Glasses: <i>ab Initio</i> Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2038-2045.	1.2	79
17	The Color and Stability of Maya Blue: TDDFT Calculations. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8683-8687.	1.5	78
18	Structural and electronic properties of modified sodium and soda-lime silicate glasses by Car ⁺ Parrinello molecular dynamics. <i>Journal of Materials Chemistry</i> , 2006, 16, 1950-1955.	6.7	73

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19	Surface Signatures of Bioactivity: MD Simulations of 45S and 65S Silicate Glasses. <i>Langmuir</i> , 2010, 26, 545-551.	1.6	73
20	Short- and medium-range structure of multicomponent bioactive glasses and melts: An assessment of the performances of shell-model and rigid-ion potentials. <i>Journal of Chemical Physics</i> , 2008, 129, 084504.	1.2	72
21	Sodium migration pathways in multicomponent silicate glasses: Carâ€™Parrinello molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2010, 133, 014701.	1.2	70
22	About the influence of lattice vibrations on the diffusion of methane in a cation-free LTA zeolite. <i>Chemical Physics Letters</i> , 1998, 296, 253-258.	1.2	69
23	O ₂ and Vacancy Diffusion on Rutile(110): Pathways and Electronic Properties. <i>ChemPhysChem</i> , 2005, 6, 1911-1916.	1.0	69
24	O ₂ Interaction and Reactivity on a Model Hydroxylated Rutile(110) Surface. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20963-20967.	1.2	67
25	Bioactive glasses as potential radioisotope vectors for in situ cancer therapy: investigating the structural effects of yttrium. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 17749.	1.3	65
26	Role of glass structure in defining the chemical dissolution behavior, bioactivity and antioxidant properties of zinc and strontium co-doped alkali-free phosphosilicate glasses. <i>Acta Biomaterialia</i> , 2014, 10, 3264-3278.	4.1	64
27	Ab Initio Molecular Dynamics Study of 45S5 Bioactive Silicate Glass. <i>Journal of Physical Chemistry B</i> , 2006, 110, 25810-25816.	1.2	62
28	First-principles string molecular dynamics: An efficient approach for finding chemical reaction pathways. <i>Journal of Chemical Physics</i> , 2004, 121, 3359-3367.	1.2	57
29	Cooling rate and size effects on the medium-range structure of multicomponent oxide glasses simulated by molecular dynamics. <i>Journal of Chemical Physics</i> , 2013, 139, 114501.	1.2	57
30	Exploring the Surface of Bioactive Glasses: Water Adsorption and Reactivity. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11936-11945.	1.5	56
31	DFT-GGA and DFT+ <i>U</i> Simulations of Thin Water Layers on Reduced TiO ₂ Anatase. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9114-9121.	1.5	56
32	Structural role of zinc in biodegradation of alkali-free bioactive glasses. <i>Journal of Materials Chemistry B</i> , 2013, 1, 3073.	2.9	54
33	Toward a Rational Design of Bioactive Glasses with Optimal Structural Features: Compositionâ€™Structure Correlations Unveiled by Solid-State NMR and MD Simulations. <i>Journal of Physical Chemistry B</i> , 2014, 118, 833-844.	1.2	54
34	Aluminosilicate Glasses As Yttrium Vectors for in situ Radiotherapy: Understanding Composition-Durability Effects through Molecular Dynamics Simulations. <i>Chemistry of Materials</i> , 2010, 22, 3725-3734.	3.2	52
35	Statics and Dynamics of Ethane Molecules in AlPO ₄ -5: A Molecular Dynamics Simulation Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 5069-5074.	6.6	44
36	Detecting Fabric Defects with a Neural Network Using Two Kinds of Optical Patterns. <i>Textile Research Journal</i> , 2002, 72, 545-550.	1.1	42

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37	The formation of nanoscale structures in soluble phosphosilicate glasses for biomedical applications: MD simulations. <i>Faraday Discussions</i> , 2007, 136, 45.	1.6	42
38	Mixed dissociated/molecular monolayer of water on the TiO ₂ (011)-(2 \bar{A} -1) surface. <i>Surface Science</i> , 2005, 591, L267-L272.	0.8	41
39	Two-step model of molecular diffusion in silicalite. <i>Journal of Chemical Physics</i> , 1999, 110, 1163-1172.	1.2	40
40	Structure and Dynamics of the Flexible Triple Helix of Water inside VPI-5 Molecular Sieves. <i>Journal of Physical Chemistry B</i> , 2002, 106, 4806-4812.	1.2	40
41	The initial stages of bioglass dissolution: a Parrinello molecular-dynamics study of the glass-water interface. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2011, 467, 2102-2111.	1.0	39
42	Electric-field-dependent empirical potentials for molecules and crystals: A first application to flexible water molecule adsorbed in zeolites. <i>Journal of Chemical Physics</i> , 2000, 112, 8267-8278.	1.2	37
43	Integrating biological activity into radioisotope vectors: molecular dynamics models of yttrium-doped bioactive glasses. <i>Journal of Materials Chemistry</i> , 2012, 22, 12023.	6.7	37
44	Diffusion and vibrational relaxation of a diatomic molecule in the pore network of a pure silica zeolite: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1996, 105, 5586-5594.	1.2	36
45	Structure and biological activity of glasses and ceramics. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2012, 370, 1271-1280.	1.6	32
46	First-Principles Molecular Dynamics Investigation of the α -Amino Acid Oxidative Half-Reaction Catalyzed by the Flavoenzyme α -Amino Acid Oxidase. <i>Biochemistry</i> , 2002, 41, 14111-14121.	1.2	28
47	Molecular dynamics simulations of a bioactive glass nanoparticle. <i>Journal of Materials Chemistry</i> , 2011, 21, 12660.	6.7	28
48	Molecular Dynamics Simulations and Structural Descriptors of Radioisotope Glass Vectors for In Situ Radiotherapy. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12614-12620.	1.2	28
49	Short-Range Structure of Yttrium Alumino-Silicate Glass for Cancer Radiotherapy: Parrinello Molecular Dynamics Simulations. <i>Advanced Engineering Materials</i> , 2010, 12, B326.	1.6	26
50	Structure-solubility relationships in fluoride-containing phosphate based bioactive glasses. <i>Journal of Materials Chemistry B</i> , 2015, 3, 9360-9373.	2.9	25
51	Influence of Calcium on the Initial Stages of the Sol-Gel Synthesis of Bioactive Glasses. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11773-11780.	1.2	25
52	Reactive molecular dynamics: an effective tool for modelling the sol-gel synthesis of bioglasses. <i>Journal of Materials Science</i> , 2017, 52, 9006-9013.	1.7	25
53	Current challenges in atomistic simulations of glasses for biomedical applications. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3874-3880.	1.3	23
54	Ab initio simulations of the structure of thin water layers on defective anatase TiO ₂ (101) surfaces. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1250-1257.	1.0	20

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55	Application of the two-step model to the diffusion of linear diatomic and triatomic molecules in silicalite. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1455-1463.	1.3	19
56	An effective harmonic potential for aluminophosphate molecular sieves: application to AlPO ₄ -5. <i>Microporous and Mesoporous Materials</i> , 2001, 42, 103-111.	2.2	17
57	Probing the fate of interstitial water in bulk bioactive glass by ab initio simulations. <i>RSC Advances</i> , 2014, 4, 36425-36436.	1.7	14
58	Realistic Models of Bioactive Glass Radioisotope Vectors in Practical Conditions: Structural Effects of Ion Exchange. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27442-27448.	1.5	13
59	Atomic-scale models of early-stage alkali depletion and SiO ₂ -rich gel formation in bioactive glasses. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2696-2702.	1.3	12
60	Molecular dynamics simulation of an activated transfer reaction in zeolites. <i>Journal of Chemical Physics</i> , 1999, 111, 5529-5543.	1.2	11
61	Hydration Effects on the Structural and Vibrational Properties of Yttrium Aluminosilicate Glasses for in Situ Radiotherapy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 14518-14528.	1.2	11
62	Two- and N-step correlated models for the analysis of molecular dynamics trajectories of linear molecules in silicalite. <i>Journal of Chemical Physics</i> , 2000, 113, 7588-7592.	1.2	9
63	The antioxidant properties of Ce-containing bioactive glass nanoparticles explained by Molecular Dynamics simulations. <i>Biomedical Glasses</i> , 2016, 2, .	2.4	9
64	A classical molecular dynamics study of recombination reactions in a microporous solid. <i>Journal of Chemical Physics</i> , 1998, 109, 2865-2873.	1.2	8
65	Recombination Reactions and Diffusive Properties of Diatomic Molecules in Two Different Microporous Structures: Silicalite and ZK4. <i>Journal of Physical Chemistry B</i> , 1999, 103, 8141-8152.	1.2	8
66	Dynamical descriptors of bioactivity: a correlation between chemical durability and ion migration in biodegradable glasses. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6334-6337.	1.3	5
67	Molecular Dynamics Methods for Modeling Complex Interactions in Biomaterials. <i>Methods in Molecular Biology</i> , 2012, 811, 285-301.	0.4	4
68	Molecular dynamics studies of chemical processes in zeolites. <i>Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics</i> , 1997, 19, 1665-1671.	0.4	3
69	Spectroscopic identification and quantitative analysis of binary mixtures using artificial neural networks. <i>Talanta</i> , 1997, 44, 1901-1909.	2.9	2
70	Rationalizing the Biodegradation of Glasses for Biomedical Applications Through Classical and Ab-initio Simulations. <i>Springer Series in Materials Science</i> , 2015, , 255-273.	0.4	2
71	Chapter 4. Molecular Dynamics Simulations of Bioactive Glass Structure and <i>In vitro</i> Reactivity. <i>RSC Smart Materials</i> , 0, , 89-104.	0.1	1
72	Computer simulations of ethane sorbed in an aluminophosphate molecular sieve. <i>Studies in Surface Science and Catalysis</i> , 2001, , 221-227.	1.5	0