

Gianluca Malavasi

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77
papers

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57
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77
ext. papers

3,876
ext. citations

5.1
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5
L-index

#	Paper	IF	Citations
77	A new self-consistent empirical interatomic potential model for oxides, silicates, and silica-based glasses. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 11780-95	3.4	362
76	Zinc-containing bioactive glasses: surface reactivity and behaviour towards endothelial cells. <i>Acta Biomaterialia</i> , 2009 , 5, 1211-22	10.8	141
75	Substitutions of cerium, gallium and zinc in ordered mesoporous bioactive glasses. <i>Acta Biomaterialia</i> , 2011 , 7, 3452-8	10.8	128
74	New Insights into the Atomic Structure of 45S5 Bioglass by Means of Solid-State NMR Spectroscopy and Accurate First-Principles Simulations. <i>Chemistry of Materials</i> , 2010 , 22, 5644-5652	9.6	112
73	Cytotoxicity of zinc-containing bioactive glasses in contact with human osteoblasts. <i>Chemico-Biological Interactions</i> , 2007 , 167, 207-18	5	108
72	Mesoporous bioactive scaffolds prepared with cerium-, gallium- and zinc-containing glasses. <i>Acta Biomaterialia</i> , 2013 , 9, 4836-44	10.8	103
71	Fluoride-containing bioactive glasses: surface reactivity in simulated body fluids solutions. <i>Acta Biomaterialia</i> , 2009 , 5, 3548-62	10.8	103
70	Insight into Elastic Properties of Binary Alkali Silicate Glasses; Prediction and Interpretation through Atomistic Simulation Techniques. <i>Chemistry of Materials</i> , 2007 , 19, 3144-3154	9.6	102
69	Molecular Dynamics Studies of Stress-Strain Behavior of Silica Glass under a Tensile Load. <i>Chemistry of Materials</i> , 2008 , 20, 4356-4366	9.6	93
68	Elucidation of the structural role of fluorine in potentially bioactive glasses by experimental and computational investigation. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 12730-9	3.4	92
67	Qualitative and quantitative structure-property relationships analysis of multicomponent potential bioglasses. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 4989-98	3.4	92
66	Evidence of catalase mimetic activity in Ce(3+)/Ce(4+) doped bioactive glasses. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4009-19	3.4	89
65	Magnesium- and strontium-co-substituted hydroxyapatite: the effects of doped-ions on the structure and chemico-physical properties. <i>Journal of Materials Science: Materials in Medicine</i> , 2012 , 23, 2867-79	4.5	85
64	Synthesis and characterization of cerium-doped glasses and in vitro evaluation of bioactivity. <i>Journal of Non-Crystalline Solids</i> , 2003 , 316, 198-216	3.9	84
63	Computational Insight into the Effect of CaO/MgO Substitution on the Structural Properties of Phospho-Silicate Bioactive Glasses. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 15723-15730	3.8	82
62	Sr-containing hydroxyapatite: morphologies of HA crystals and bioactivity on osteoblast cells. <i>Materials Science and Engineering C</i> , 2013 , 33, 1132-42	8.3	81
61	Role of Magnesium in Soda-Lime Glasses: Insight into Structural, Transport, and Mechanical Properties through Computer Simulations. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 11034-11041	3.8	73

60	In vitro antibacterial capacity and cytocompatibility of SiO-CaO-PO meso-macroporous glass scaffolds enriched with ZnO. <i>Journal of Materials Chemistry B</i> , 2014 , 2, 4836-4847	7.3	70
59	Synthesis, Characterization, and Molecular Dynamics Simulation Of Na ₂ O-CaO-BiO ₂ -ZnO Glasses. <i>Journal of Physical Chemistry B</i> , 2002 , 106, 9753-9760	3.4	68
58	Quantitative structure-property relationships of potentially bioactive fluoro phospho-silicate glasses. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 10331-8	3.4	67
57	FFSiOH: a New Force Field for Silica Polymorphs and Their Hydroxylated Surfaces Based on Periodic B3LYP Calculations. <i>Chemistry of Materials</i> , 2008 , 20, 2522-2531	9.6	65
56	In vitro and in vivo behaviour of zinc-doped phosphosilicate glasses. <i>Acta Biomaterialia</i> , 2009 , 5, 419-28	10.8	64
55	Structural and in vitro study of cerium, gallium and zinc containing sol-gel bioactive glasses. <i>Journal of Materials Chemistry</i> , 2012 , 22, 13698		60
54	Void size distribution in MD-modelled silica glass structures. <i>Journal of Non-Crystalline Solids</i> , 2006 , 352, 285-296	3.9	58
53	Study of the structural role of gallium and aluminum in 45S5 bioactive glasses by molecular dynamics simulations. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 4142-50	3.4	55
52	Medium-range order in phospho-silicate bioactive glasses: Insights from MAS-NMR spectra, chemical durability experiments and molecular dynamics simulations. <i>Journal of Non-Crystalline Solids</i> , 2008 , 354, 84-89	3.9	50
51	Curcumin release from cerium, gallium and zinc containing mesoporous bioactive glasses. <i>Microporous and Mesoporous Materials</i> , 2013 , 180, 92-101	5.3	48
50	Properties of zinc releasing surfaces for clinical applications. <i>Journal of Biomaterials Applications</i> , 2008 , 22, 505-26	2.9	46
49	Removal of cadmium ion by means of synthetic hydroxyapatite. <i>Waste Management</i> , 2002 , 22, 853-7	8.6	43
48	Elastic and dynamical properties of alkali-silicate glasses from computer simulations techniques. <i>Theoretical Chemistry Accounts</i> , 2008 , 120, 557-564	1.9	40
47	Gallium-containing phospho-silicate glasses: synthesis and in vitro bioactivity. <i>Materials Science and Engineering C</i> , 2012 , 32, 1401-6	8.3	36
46	Fluoride-containing bioactive glasses inhibit pentose phosphate oxidative pathway and glucose 6-phosphate dehydrogenase activity in human osteoblasts. <i>Chemico-Biological Interactions</i> , 2010 , 183, 405-15	5	34
45	The effect of composition on structural, thermal, redox and bioactive properties of Ce-containing glasses. <i>Materials and Design</i> , 2016 , 97, 73-85	8.1	33
44	Cerium-doped bioactive 45S5 glasses: spectroscopic, redox, bioactivity and biocatalytic properties. <i>Journal of Materials Science</i> , 2017 , 52, 8845-8857	4.3	31
43	First-principles simulations of the ²⁷ Al and ¹⁷ O solid-state NMR spectra of the CaAl ₂ Si ₃ O ₁₀ glass. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	31

42	An ab initio parameterized interatomic force field for hydroxyapatite. <i>Journal of Materials Chemistry</i> , 2007 , 17, 2061		31
41	Thermodynamic aspects of the adsorption of hexametaphosphate on kaolinite. <i>Journal of Colloid and Interface Science</i> , 2005 , 292, 322-9	9.3	31
40	On the dissolution/reaction of small-grain Bioglass [®] 45S5 and F-modified bioactive glasses in artificial saliva (AS). <i>Applied Surface Science</i> , 2011 , 257, 4185-4195	6.7	30
39	A computational multiscale strategy to the study of amorphous materials. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 933-942	1.9	29
38	A computational tool for the prediction of crystalline phases obtained from controlled crystallization of glasses. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 21586-92	3.4	29
37	Functionalization of sol gel bioactive glasses carrying Au nanoparticles: selective Au affinity for amino and thiol ligand groups. <i>Langmuir</i> , 2010 , 26, 18600-5	4	28
36	Bioactive glasses containing Au nanoparticles. Effect of calcination temperature on structure, morphology, and surface properties. <i>Langmuir</i> , 2010 , 26, 10303-14	4	28
35	The role of coordination chemistry in the development of innovative gallium-based bioceramics: the case of curcumin. <i>Journal of Materials Chemistry</i> , 2011 , 21, 5027		25
34	Molecular dynamics simulations of sodium silicate glasses: Optimization and limits of the computational procedure. <i>Computational Materials Science</i> , 2010 , 47, 739-751	3.2	23
33	Influence of the Chemical Composition on Nature and Activity of the Surface Layer of Zn-Substituted Sol-Gel (Bioactive) Glasses. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 2196-2210	3.8	22
32	Synthesis and characterization of bioactive glasses functionalized with Cu nanoparticles and organic molecules. <i>Journal of the European Ceramic Society</i> , 2012 , 32, 2777-2783	6	21
31	A combined experimental and computational approach to (Na ₂ O) _{1-x} CaO _x (ZnO) _x 2SiO ₂ glasses characterization. <i>Journal of Non-Crystalline Solids</i> , 2004 , 345-346, 710-714	3.9	21
30	Highly-Bioreactive Silica-Based Mesoporous Bioactive Glasses Enriched with Gallium(III). <i>Materials</i> , 2018 , 11,	3.5	20
29	New formulation of functionalized bioactive glasses to be used as carriers for the development of pH-stimuli responsive biomaterials for bone diseases. <i>Langmuir</i> , 2014 , 30, 4703-15	4	19
28	Towards the controlled release of metal nanoparticles from biomaterials: Physico-chemical, morphological and bioactivity features of Cu-containing sol-gel glasses. <i>Applied Surface Science</i> , 2013 , 283, 240-248	6.7	19
27	Towards a quantitative rationalization of multicomponent glass properties by means of molecular dynamics simulations. <i>Molecular Simulation</i> , 2006 , 32, 1045-1055	2	19
26	Gallium-containing phosphosilicate glasses: functionalization and in-vitro bioactivity. <i>Materials Science and Engineering C</i> , 2013 , 33, 3190-6	8.3	18
25	Deflocculant effects on the surface properties of kaolinite investigated through malachite green adsorption. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2008 , 329, 31-37	5.1	18

24	Crystallization kinetics of bioactive glasses in the ZnO-Na ₂ O-CaO-SiO ₂ system. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 8401-8	2.8	17
23	Multitechnique approach to V ₂ O ₅ /SiO ₄ pigment characterization and synthesis optimization. <i>Journal of the European Ceramic Society</i> , 2007 , 27, 1743-1750	6	17
22	Ga-Modified (SiO ₂ -CaO) Sol-Gel Glasses: Possible Relationships between Surface Chemical Properties and Bioactivity. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 22461-22474	3.8	16
21	New insights into the bioactivity of SiO ₂ -CaO and SiO ₂ -CaO-P ₂ O ₅ sol-gel glasses by molecular dynamics simulations. <i>Journal of Sol-Gel Science and Technology</i> , 2013 , 67, 208-219	2.3	15
20	The toxic effect of fluoride on MG-63 osteoblast cells is also dependent on the production of nitric oxide. <i>Chemico-Biological Interactions</i> , 2011 , 190, 179-86	5	15
19	Cytocompatibility of Potential Bioactive Cerium-Doped Glasses based on 45S5. <i>Materials</i> , 2019 , 12,	3.5	14
18	Gold-containing bioactive glasses: a solid-state synthesis to produce alternative biomaterials for bone implantations. <i>Journal of the Royal Society Interface</i> , 2013 , 10, 20121040	4.1	14
17	Novel bio-conjugate materials: soybean peroxidase immobilized on bioactive glasses containing Au nanoparticles. <i>Journal of Materials Chemistry</i> , 2011 , 21, 10970		13
16	Structure of active cerium sites within bioactive glasses. <i>Journal of the American Ceramic Society</i> , 2017 , 100, 5086-5095	3.8	12
15	Density of multicomponent silica-based potential bioglasses: Quantitative structure-property relationships (QSPR) analysis. <i>Journal of the European Ceramic Society</i> , 2007 , 27, 499-504	6	12
14	Mesoporous bioactive glasses doped with cerium: Investigation over enzymatic-like mimetic activities and bioactivity. <i>Ceramics International</i> , 2019 , 45, 20910-20920	5.1	10
13	SiO ₂ -CaO-P ₂ O ₅ Bioactive Glasses: A Promising Curcuminoids Delivery System. <i>Materials</i> , 2016 , 9,	3.5	9
12	Cerium Containing Bioactive Glasses: A Review. <i>ACS Biomaterials Science and Engineering</i> , 2021 , 7, 4388-4401	5.9	8
11	Cell Proliferation to Evaluate Preliminarily the Presence of Enduring Self-Regenerative Antioxidant Activity in Cerium Doped Bioactive Glasses. <i>Materials</i> , 2020 , 13,	3.5	6
10	Conjugation of amino-bioactive glasses with 5-aminofluorescein as probe molecule for the development of pH sensitive stimuli-responsive biomaterials. <i>Journal of Materials Science: Materials in Medicine</i> , 2014 , 25, 2243-53	4.5	6
9	Evaluation of the behaviour of fluorine-containing bioactive glasses: reactivity in a simulated body fluid solution assisted by multivariate data analysis. <i>Journal of Materials Science: Materials in Medicine</i> , 2012 , 23, 639-48	4.5	5
8	Systematic investigation of the parameters that influence the luminescence properties of photoluminescent pigments. <i>Journal of Luminescence</i> , 2016 , 175, 141-148	3.8	5
7	An atomic-level look at the structure-property relationship of cerium-doped glasses using classical molecular dynamics. <i>Journal of Non-Crystalline Solids</i> , 2018 , 498, 331-337	3.9	4

6	Composition and morphology effects on catalase mimetic activity of potential bioactive glasses. <i>Ceramics International</i> , 2020 , 46, 25854-25864	5.1	4
5	Preparation and Luminescence Properties of BaSiO ₃ Long Persistent Phosphors Doped with Rare-Earth Elements. <i>Materials</i> , 2019 , 12,	3.5	4
4	Synthesis and Characterisation of Strontium and Magnesium Co-Substituted Biphasic Calcium Phosphates. <i>Key Engineering Materials</i> , 2012 , 529-530, 88-93	0.4	3
3	Role of cerium oxide in bioactive glasses during catalytic dissociation of hydrogen peroxide. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 23507-23514	3.6	2
2	The effect of the incorporation of catalase mimetic activity cations on the structural, thermal and chemical durability properties of the 45S5 Bioglass [®] . <i>Acta Materialia</i> , 2022 , 229, 117801	8.4	0
1	First-principles simulations of the ²⁷ Al and ¹⁷ O solid-state NMR spectra of the CaAl ₂ Si ₃ O ₁₀ glass. <i>Highlights in Theoretical Chemistry</i> , 2013 , 87-97		