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List of Publications by Year in descending order

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27
papers

652
citations

567281

15
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g-index

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all docs

29
docs citations

29
times ranked

649
citing authors

#	ARTICLE	IF	CITATIONS
1	Carbon dioxide and water incorporation mechanisms in SrFeO ₃ phases: a computational study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25146-25155.	2.8	4
2	Atomic-scale clustering inhibits the bioactivity of fluoridated phosphate glasses. <i>Biomedical Glasses</i> , 2019, 5, 76-84.	2.4	5
3	Atomic structure of Mg-based metallic glasses from molecular dynamics and neutron diffraction. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8504-8515.	2.8	21
4	Effect of strontium inclusion on the bioactivity of phosphate-based glasses. <i>Journal of Materials Science</i> , 2017, 52, 9014-9022.	3.7	21
5	Atomic structure and dissolution properties of yttrium-containing phosphate glasses. <i>International Journal of Applied Glass Science</i> , 2017, 8, 412-417.	2.0	10
6	Structures and properties of phosphate-based bioactive glasses from computer simulation: a review. <i>Journal of Materials Chemistry B</i> , 2017, 5, 5297-5306.	5.8	19
7	Bioactive Sol-Gel Glasses at the Atomic Scale: The Complementary Use of Advanced Probe and Computer Modeling Methods. <i>International Journal of Applied Glass Science</i> , 2016, 7, 147-153.	2.0	9
8	Investigating structural features which control the dissolution of bioactive phosphate glasses: Beyond the network connectivity. <i>Journal of Non-Crystalline Solids</i> , 2016, 432, 31-34.	3.1	46
9	Atomic structure of biodegradable Mg-based bulk metallic glass. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12894-12898.	2.8	12
10	Properties of water confined in hydroxyapatite nanopores as derived from molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	22
11	Ab initio molecular dynamics simulations of structural changes associated with the incorporation of fluorine in bioactive phosphate glasses. <i>Biomaterials</i> , 2014, 35, 6164-6171.	11.4	42
12	On the structure of biomedical silver-doped phosphate-based glasses from molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21135-21143.	2.8	12
13	Nanoscale Chains Control the Solubility of Phosphate Glasses for Biomedical Applications. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10652-10657.	2.6	33
14	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
15	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.	2.6	28
16	Polarizable force field development and molecular dynamics study of phosphate-based glasses. <i>Journal of Chemical Physics</i> , 2012, 137, 234502.	3.0	33
17	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.	2.8	65
18	Fluorine Environment in Bioactive Glasses: <i>Ab Initio</i> Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2038-2045.	2.6	79

#	ARTICLE	IF	CITATIONS
19	Structural properties and phase transitions in a silica clathrate. Journal of Chemical Physics, 2011, 134, 074506.	3.0	5
20	Short-Range Structure of Yttrium Alumino-Silicate Glass for Cancer Radiotherapy: Car Parrinello Molecular Dynamics Simulations. Advanced Engineering Materials, 2010, 12, B326.	3.5	26
21	Aluminosilicate Glasses As Yttrium Vectors for in situ Radiotherapy: Understanding Composition-Durability Effects through Molecular Dynamics Simulations. Chemistry of Materials, 2010, 22, 3725-3734.	6.7	52
22	Polarizable interatomic force field for TiO_2 using density functional theory. Physical Review B, 2010, 81, .	3.2	27
23	Vibrational behavior of a realistic amorphous-silicon model. Journal of Non-Crystalline Solids, 2007, 353, 2272-2279.	3.1	10
24	Modeling the atomic structure of very high-density amorphous ice. Physical Review B, 2005, 72, .	3.2	13
25	Structural characteristics of positionally disordered lattices: Relation to the first sharp diffraction peak in glasses. Physical Review B, 2004, 70, .	3.2	13
26	Atomic vibrations in disordered systems: Comparison of disordered diamond lattices and a realistic amorphous silicon model. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 2904-2907.	0.8	2
27	Positional disorder in lattices: a model for the structural order responsible for the first sharp diffraction peak in glasses. Journal of Physics Condensed Matter, 2004, 16, S5109-S5120.	1.8	5