

Jean-Marc Delaye

List of Publications by Year in descending order

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36
papers

1,045
citations

471509

17
h-index

414414

32
g-index

36
all docs

36
docs citations

36
times ranked

781
citing authors

#	ARTICLE	IF	CITATIONS
1	Deciphering the non-linear impact of Al on chemical durability of silicate glass. <i>Acta Materialia</i> , 2022, 225, 117478.	7.9	17
2	Behaviors of sodium and calcium ions at the borosilicate glass-water interface: Gaining new insights through an <i>ab initio</i> molecular dynamics study. <i>Journal of Chemical Physics</i> , 2022, 156, 134501.	3.0	14
3	Development of potentials for molecular dynamics simulations of dry and hydrated calcium aluminosilicate glasses by force matching and refinement. <i>Journal of Non-Crystalline Solids</i> , 2022, 592, 121746.	3.1	4
4	A classical molecular dynamics simulation method for the formation of "dry" gels from boro-aluminosilicate glass structures. <i>Journal of Non-Crystalline Solids</i> , 2021, 553, 120513.	3.1	3
5	Atomic Insights into the Events Governing the Borosilicate Glass-water Interface. <i>Journal of Physical Chemistry C</i> , 2021, 125, 7919-7931.	3.1	20
6	Impact of magnesium on the structure of aluminoborosilicate glasses: A solid-state NMR and Raman spectroscopy study. <i>Journal of the American Ceramic Society</i> , 2021, 104, 4518-4536.	3.8	26
7	Predicting the dissolution rate of borosilicate glasses using QSPR analysis based on molecular dynamics simulations. <i>Journal of the American Ceramic Society</i> , 2021, 104, 4445-4458.	3.8	18
8	Investigation of alumino-silicate glasses by coupling experiments and simulations: Part I - Structures. <i>Journal of Non-Crystalline Solids</i> , 2021, 567, 120936.	3.1	3
9	Investigation of alumino-silicate glasses by coupling experiments and simulations: Part II - radiation effects. <i>Journal of Non-Crystalline Solids</i> , 2021, 569, 120969.	3.1	3
10	Influence of Magnesium on the Structure of Complex Multicomponent Silicates: Insights from Molecular Simulations and Neutron Scattering Experiments. <i>Journal of Physical Chemistry B</i> , 2021, 125, 11761-11776.	2.6	9
11	Leaching and Reactivity at the Sodium Aluminosilicate Glass-water Interface: Insights from a ReaxFF Molecular Dynamics Study. <i>Journal of Physical Chemistry C</i> , 2021, 125, 27170-27184.	3.1	21
12	Molecular dynamics simulation of ballistic effects in mesoporous silica. <i>Journal of Non-Crystalline Solids</i> , 2020, 549, 120346.	3.1	2
13	NMR shifts in aluminosilicate glasses <i>via</i> machine learning. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 21709-21725.	2.8	25
14	Monte Carlo simulation of the corrosion of irradiated simplified nuclear waste glasses. <i>Journal of Non-Crystalline Solids</i> , 2019, 519, 119449.	3.1	13
15	Comparing the reactivity of glasses with their crystalline equivalents: The case study of plagioclase feldspar. <i>Geochimica Et Cosmochimica Acta</i> , 2019, 254, 122-141.	3.9	27
16	Many-body effects at the origin of structural transitions in B ₂ O ₃ . <i>Journal of Chemical Physics</i> , 2019, 151, 224508.	3.0	3
17	Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses. <i>Journal of Non-Crystalline Solids</i> , 2019, 505, 188-201.	3.1	16
18	Structural study of Na ₂ O-B ₂ O ₃ -SiO ₂ -La ₂ O ₃ glasses from molecular simulations using a polarizable force field. <i>Journal of Non-Crystalline Solids</i> , 2018, 499, 371-379.	3.1	16

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19	Raman spectra of indented pristine and irradiated sodium borosilicate glasses. Journal of Non-Crystalline Solids, 2017, 464, 5-13.	3.1	18
20	Drivers of Water Transport in Glass: Chemical or Topological Effect of the Glass Network?. Journal of Physical Chemistry C, 2017, 121, 16201-16215.	3.1	15
21	Structural study of Na ₂ O-B ₂ O ₃ -SiO ₂ glasses from molecular simulations using a polarizable force field. Journal of Chemical Physics, 2017, 147, 161711.	3.0	34
22	From network depolymerization to stress corrosion cracking in sodium-borosilicate glasses: Effect of the chemical composition. Journal of Non-Crystalline Solids, 2016, 450, 174-184.	3.1	16
23	Nanoindentation studies of simplified nuclear glasses using molecular dynamics. Journal of Non-Crystalline Solids, 2014, 401, 147-153.	3.1	29
24	Nanoindentation of pristine and disordered silica: Molecular Dynamics simulations. Journal of Non-Crystalline Solids, 2013, 382, 87-94.	3.1	24
25	SiO ₂ -Na ₂ O-B ₂ O ₃ density: A comparison of experiments, simulations, and theory. Journal of Non-Crystalline Solids, 2013, 382, 32-44.	3.1	51
26	Topological analysis of the structure of self-irradiated sodium borosilicate glass. Journal of Non-Crystalline Solids, 2012, 358, 3427-3432.	3.1	9
27	Modeling the effect of composition and thermal quenching on the fracture behavior of borosilicate glass. Journal of Non-Crystalline Solids, 2012, 358, 3268-3279.	3.1	30
28	Molecular dynamics simulation of radiation damage in glasses. Journal of Non-Crystalline Solids, 2011, 357, 2763-2768.	3.1	79
29	Development of empirical potentials for sodium borosilicate glass systems. Journal of Non-Crystalline Solids, 2011, 357, 3313-3321.	3.1	125
30	Contribution of first-principles calculations to multinuclear NMR analysis of borosilicate glasses. Magnetic Resonance in Chemistry, 2010, 48, S159-S170.	1.9	49
31	Surface of a calcium aluminosilicate glass by classical and ab initio molecular dynamics simulations. Surface Science, 2008, 602, 114-125.	1.9	17
32	Evolution of the local environment of lanthanum during simplified SON68 glass leaching. Journal of Non-Crystalline Solids, 2007, 353, 344-353.	3.1	10
33	Damage inhomogeneity in the core region of displacement cascades in simplified nuclear glasses. Journal of Nuclear Materials, 2006, 348, 243-255.	2.7	14
34	Structural properties of a calcium aluminosilicate glass from molecular-dynamics simulations: A finite size effects study. Journal of Chemical Physics, 2004, 120, 10172-10181.	3.0	101
35	Chemical dependence of network topology of calcium aluminosilicate glasses: a computer simulation study. Journal of Non-Crystalline Solids, 2003, 332, 255-270.	3.1	149
36	Molecular dynamics study of the structure and dynamic behavior at the surface of a silicate glass. Journal of Non-Crystalline Solids, 2003, 315, 187-196.	3.1	35