Jean-Marc Delaye

List of Publications by Year
in descending order

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	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
2	Development of empirical potentials for sodium borosilicate glass systems. Journal of Non-Crystalline Solids, 2011, 357, 3313-3321.	3.1	125
3	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
4	Molecular dynamics simulation of radiation damage in glasses. Journal of Non-Crystalline Solids, 2011, 357, 2763-2768.	3.1	79
5	SiO2â€“Na2Oâ€“B2O3 density: A comparison of experiments, simulations, and theory. Journal of Non-Crystalline Solids, 2013, 382, 32-44.	3.1	51
6	Contribution of first-principles calculations to multinuclear NMR analysis of borosilicate glasses. Magnetic Resonance in Chemistry, 2010, 48, S159-S170.	1.9	49
7	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
8	Structural study of Na2Oâ€“B2O3â€“SiO2 glasses from molecular simulations using a polarizable force field. Journal of Chemical Physics, 2017, 147, 161711.	3.0	34
9	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
10	Nanoindentation studies of simplified nuclear glasses using molecular dynamics. Journal of Non-Crystalline Solids, 2014, 401, 147-153.	3.1	29
11	Comparing the reactivity of glasses with their crystalline equivalents: The case study of plagioclase feldspar. Geochimica Et Cosmochimica Acta, 2019, 254, 122-141.	3.9	27
12	Impact of magnesium on the structure of aluminoborosilicate glasses: A solidâ€state NMR and Raman spectroscopy study. Journal of the American Ceramic Society, 2021, 104, 4518-4536.	3.8	26
13	NMR shifts in aluminosilicate glasses via machine learning. Physical Chemistry Chemical Physics, 2019, 21, 21709-21725.	2.8	25
14	Nanoindentation of pristine and disordered silica: Molecular Dynamics simulations. Journal of Non-Crystalline Solids, 2013, 382, 87-94.	3.1	24
15	Leaching and Reactivity at the Sodium Aluminosilicate Glassâ€“Water Interface: Insights from a ReaxFF Molecular Dynamics Study. Journal of Physical Chemistry C, 2021, 125, 27170-27184.	3.1	21
16	Atomic Insights into the Events Governing the Borosilicate Glassâ€“Water Interface. Journal of Physical Chemistry C, 2021, 125, 7919-7931.	3.1	20
17	Raman spectra of indented pristine and irradiated sodium borosilicateÂglasses. Journal of Non-Crystalline Solids, 2017, 464, 5-13.	3.1	18
18	Predicting the dissolution rate of borosilicate glasses using QSPR analysis based on molecular dynamics simulations. Journal of the American Ceramic Society, 2021, 104, 4445-4458.	3.8	18

#	Article	IF	Citations
19	Surface of a calcium aluminosilicate glass by classical and ab initio molecular dynamics simulations. Surface Science, 2008, 602, 114-125.	1.9	17
20	Deciphering the non-linear impact of Al on chemical durability of silicate glass. Acta Materialia, 2022, 225, 117478.	7.9	17
21	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
22	Structural study of Na2O-B2O3-SiO2-La2O3 glasses from molecular simulations using a polarizable force field. Journal of Non-Crystalline Solids, 2018, 499, 371-379.	3.1	16
23	Molecular dynamics simulation of ballistic effects in simplified nuclear waste glasses. Journal of Non-Crystalline Solids, 2019, 505, 188-201.	3.1	16
24	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
25	Damage inhomogeneity in the core region of displacement cascades in simplified nuclear glasses. Journal of Nuclear Materials, 2006, 348, 243-255.	2.7	14
26	Behaviors of sodium and calcium ions at the borosilicate glassâ€“water interface: Gaining new insights through an ab initio molecular dynamics study. Journal of Chemical Physics, 2022, 156, 134501.	3.0	14
27	Monte Carlo simulation of the corrosion of irradiated simplified nuclear waste glasses. Journal of Non-Crystalline Solids, 2019, 519, 119449.	3.1	13
28	Evolution of the local environment of lanthanum during simplified SON68 glass leaching. Journal of Non-Crystalline Solids, 2007, 353, 344-353.	3.1	10
29	Topological analysis of the structure of self-irradiated sodium borosilicate glass. Journal of Non-Crystalline Solids, 2012, 358, 3427-3432.	3.1	9
30	Influence of Magnesium on the Structure of Complex Multicomponent Silicates: Insights from Molecular Simulations and Neutron Scattering Experiments. Journal of Physical Chemistry B, 2021, 125, 11761-11776.	2.6	9
31	Development of potentials for molecular dynamics simulations of dry and hydrated calcium aluminosilicate glasses by force matching and refinement. Journal of Non-Crystalline Solids, 2022, 592, 121746.	3.1	4
32	Many-body effects at the origin of structural transitions in B2O3. Journal of Chemical Physics, 2019, 151, 224508.	3.0	3
33	A classical molecular dynamics simulation method for the formation of â€œdryâ€•gels from boro-aluminosilicate glass structures. Journal of Non-Crystalline Solids, 2021, 553, 120513.	3.1	3
34	Investigation of alumino-silicate glasses by coupling experiments and simulations: Part I - Structures. Journal of Non-Crystalline Solids, 2021, 567, 120936.	3.1	3
35	Investigation of alumino-silicate glasses by coupling experiments and simulations: Part II - radiation effects. Journal of Non-Crystalline Solids, 2021, 569, 120969.	3.1	3
36	Molecular dynamics simulation of ballistic effects in mesoporous silica. Journal of Non-Crystalline Solids, 2020, 549, 120346.	3.1	2