FrÃ©dÃ©ric Affouard

List of Publications by Year
in descending order

94 papers	2,614 citations	159358 30 h-index	197535 49 g-index
96 all docs	96 docs citations	96 times ranked	2425 citing authors

#	Article	IF	Citations
1	How Homogeneous Are the Trehalose, Maltose, and Sucrose Water Solutions? An Insight from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 11046-11057.	1.2	226
2	Molecular Motions in Amorphous Ibuprofen As Studied by Broadband Dielectric Spectroscopy. Journal of Physical Chemistry B, 2008, 112, 11087-11099.	1.2	152
3	Does the Interaction Potential Determine Both the Fragility of a Liquid and the Vibrational Properties of Its Glassy State?. Physical Review Letters, 2004, 93, 105502.	2.9	128
4	Comparative study of trehalose, sucrose and maltose in water solutions by molecular modelling. Europhysics Letters, 2004, 65, 41-47.	0.7	112
5	How Do Trehalose, Maltose, and Sucrose Influence Some Structural and Dynamical Properties of Lysozyme? Insight from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 9410-9420.	1.2	110
6	Influence of homologous disaccharides on the hydrogen-bond network of water: complementary Raman scattering experiments and molecular dynamics simulations. Carbohydrate Research, 2005, 340, 881-887.	1.1	105
7	Evidence of a two-stage thermal denaturation process in lysozyme: A Raman scattering and differential scanning calorimetry investigation. Journal of Chemical Physics, 2006, 124, 014703.	1.2	83
8	Thermostabilization Mechanism of Bovine Serum Albumin by Trehalose. Journal of Physical Chemistry B, 2009, 113, 6119-6126.	1.2	75
9	Analysis of Sugar Bioprotective Mechanisms on the Thermal Denaturation of Lysozyme from Raman Scattering and Differential Scanning Calorimetry Investigations. Journal of Physical Chemistry B, 2006, 110, 22886-22893.	1.2	70
10	The breakdown of the Stokesâ€“Einstein relation in supercooled binary liquids. Journal of Physics Condensed Matter, 2003, 15, 5397-5407.	0.7	62
11	Dependence of the fragility of a glass former on the softness of interparticle interactions. Journal of Chemical Physics, 2011, 135, 194503.	1.2	59
12	How Strongly Does Trehalose Interact with Lysozyme in the Solid State? Insights from Molecular Dynamics Simulation and Inelastic Neutron Scattering. Journal of Physical Chemistry B, 2012, 116, 11103-11116.	1.2	58
13	Molecular dynamics of model liquid crystals composed of semiflexible molecules. Physical Review E, 1996, 54, 5178-5186.	0.8	56
14	Thermal Denaturation of Beta-Lactoglobulin and Stabilization Mechanism by Trehalose Analyzed from Raman Spectroscopy Investigations. Journal of Physical Chemistry B, 2010, 114, 6675-6684.	1.2	56
15	A combined neutron scattering and simulation study on bioprotectant systems. Chemical Physics, 2005, 317, 258-266.	0.9	52
16	Molecular dynamics simulations of glycerol glass-forming liquid. Chemical Physics, 2005, 317, 253-257.	0.9	51
17	Ab initio structure determination of phase II of racemic ibuprofen by X-ray powder diffraction. Acta Crystallographica Section B: Structural Science, 2010, 66, 76-80.	1.8	50
18	Ab initio structure determination of the high-temperature phase of anhydrous caffeine by X-ray powder diffraction. Acta Crystallographica Section B: Structural Science, 2005, 61, 329-334.	1.8	49

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19	Slowing down of water dynamics in disaccharide aqueous solutions. Journal of Non-Crystalline Solids, 2011, 357, 695-699.	1.5	49
20	Influence of Nanoscale Confinement on the Molecular Mobility of Ibuprofen. Journal of Physical Chemistry C, 2014, 118, 13857-13868.	1.5	49
21	Structure determination of the stable anhydrous phase of Î±-lactose from X-ray powder diffraction. Acta Crystallographica Section B: Structural Science, 2005, 61, 185-191.	1.8	43
22	Molecular dynamics simulation of nanoconfined glycerol. Physical Chemistry Chemical Physics, 2009, 11, 11127.	1.3	43
23	Molecular Mobility of AmorphousS-Flurbiprofen: A Dielectric Relaxation Spectroscopy Approach. Molecular Pharmaceutics, 2014, 11, 112-130.	2.3	38
24	Ab initio structure determination of the hygroscopic anhydrous form of Î±-lactose by powder X-ray diffraction. Acta Crystallographica Section B: Structural Science, 2004, 60, 453-460.	1.8	35
25	A Monte Carlo study of metastable structures of the cyanoadamantane crystal. Journal of Chemical Physics, 1998, 109, 6753-6763.	1.2	33
26	Molecular Mobility in Amorphous Biobased Poly(ethylene 2,5-furandicarboxylate) and Poly(ethylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.2	33
27	Structure determination of the 1/1 Î±/Î² mixed lactose by X-ray powder diffraction. Acta Crystallographica Section B: Structural Science, 2005, 61, 455-463.	1.8	32
28	Study of the relaxational and vibrational dynamics of bioprotectant glass-forming mixtures by neutron scattering and molecular dynamics simulation. Journal of Chemical Physics, 2010, 132, 184512.	1.2	32
29	Is There Something of Mode Coupling Theory in Orientationally Disordered Crystals?. Physical Review Letters, 2001, 87, 035501.	2.9	30
30	Sugar bioprotective effects on thermal denaturation of lysozyme: Insights from Raman scattering experiments and molecular dynamics simulation. Journal of Non-Crystalline Solids, 2006, 352, 4430-4436.	1.5	30
31	Low-frequency vibrational properties of lysozyme in sugar aqueous solutions: A Raman scattering and molecular dynamics simulation study. Journal of Chemical Physics, 2009, 131, 245103.	1.2	30
32	Molecular dynamics simulations of lysozyme in water/sugar solutions. Chemical Physics, 2008, 345, 267-274.	0.9	28
33	Breakdown of the Stokesâ€“Einstein relation in Lennard-Jones glassforming mixtures with different interaction potential. Journal of Chemical Physics, 2009, 131, 104510.	1.2	28
34	Orientationally disordered crystals: from the onset of slow dynamics to the glass transition. Journal of Non-Crystalline Solids, 2002, 307-310, 9-15.	1.5	27
35	Debye Process in Ibuprofen Glass-Forming Liquid: Insights from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2010, 114, 11397-11402.	1.2	26
36	Affinity prediction computations and mechanosynthesis of carbamazepine based cocrystals. CrystEngComm, 2019, 21, 6991-7001.	1.3	26

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37	Characterization of molecular motions in biomolecular systems by elastic incoherent neutron scattering. Journal of Chemical Physics, 2008, 129, 155103.	1.2	25
38	Subterahertz characterization of ethanol hydration layers by microfluidic system. Applied Physics Letters, 2010, 97, .	1.5	24
39	Molecular mobility of amorphous N-acetyl-Î±-methylbenzylamine and Debye relaxation evidenced by dielectric relaxation spectroscopy and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2019, 21, 702-717.	1.3	23
40	Molecular Packing, Hydrogen Bonding, and Fast Dynamics in Lysozyme/Trehalose/Glycerol and Trehalose/Glycerol Glasses at Low Hydration. Journal of Physical Chemistry B, 2017, 121, 9437-9451.	1.2	22
41	Experimental and numerical signatures of dynamical crossover in orientationally disordered crystals. Europhysics Letters, 2001, 53, 611-617.	0.7	21
42	Mixing effects in glass-forming Lennard-Jones mixtures. Journal of Chemical Physics, 2009, 130, 154505.	1.2	21
43	Predictive Calculation of the Crystallization Tendency of Model Pharmaceuticals in the Supercooled State from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 10768-10783.	1.2	20
44	Highly sensitive terahertz spectroscopy in microsystem. RSC Advances, 2012, 2, 10064.	1.7	18
45	Terahertz microfluidic sensor for in situ exploration of hydration shell of molecules. Chemometrics and Intelligent Laboratory Systems, 2013, 123, 28-35.	1.8	18
46	Indication for a change of dynamics in plastic crystal chloroadamantane: Raman scattering experiment and molecular dynamics simulation. Journal of Physics Condensed Matter, 2001, 13, 7237-7248.	0.7	16
47	Microscopic description of protein thermostabilization mechanisms with disaccharides from Raman spectroscopy investigations. Journal of Physics Condensed Matter, 2007, 19, 205142.	0.7	16
48	Metastable state in glassy crystal cyanoadamantane: experiments and simulations. Journal of Non-Crystalline Solids, 1998, 235-237, 559-566.	1.5	15
49	Onset of slow dynamics in difluorotetrachloroethane glassy crystal. Journal of Chemical Physics, 2005, 123, 084501.	1.2	15
50	Analogy of the slow dynamics between the supercooled liquid and supercooled plastic crystal states of difluorotetrachloroethane. Physical Review E, 2005, 72, 012501.	0.8	14
51	Two-step rotational relaxation in glassy crystal cyanoadamantane. Physical Review B, 1999, 59, R9011-R9014.	1.1	13
52	Molecular dynamics investigations of glassforming binary Lennard-Jones systems with different anharmonicities. Journal of Non-Crystalline Solids, 2006, 352, 4630-4634.	1.5	13
53	Effect of anharmonicity on the diffusion in glassforming binary Lennard-Jones systems. Journal of Non-Crystalline Solids, 2007, 353, 3924-3927.	1.5	13
54	Raman effects under pressure in chloroadamantane plastic crystal. Journal of Physics Condensed Matter, 2002, 14, 8725-8741.	0.7	11

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55	The non-Gaussian dynamics of glycerol. Journal of Physics Condensed Matter, 2011, 23, 505102.	0.7	10
56	Local molecular organizations of ibuprofen, flurbiprofen and ketoprofen in the liquid phase: Insights from molecular dynamics simulations. Journal of Molecular Liquids, 2015, 205, 74-77.	2.3	10
57	Structure determination of <scp>L</scp>-arabinitol by powder X-ray diffraction. Acta Crystallographica Section B: Structural Science, 2012, 68, 407-411.	1.8	9
58	A comparative study of ibuprofen and ketoprofen glass-forming liquids by molecular dynamics simulations. Journal of Chemical Physics, 2015, 143, 164506.	1.2	9
59	Impact of chirality on peculiar ibuprofen molecular dynamics: hydrogen bonding organization and syn vs. anti carboxylic group conformations. Physical Chemistry Chemical Physics, 2018, 20, 29528-29538.	1.3	9
60	A molecular-dynamics simulation of the orientational melting of potassium perchlorate. Europhysics Letters, 1996, 33, 365-370.	0.7	6
61	Lactulose: A Model System to Investigate Solid State Amorphization Induced by Milling. Journal of Pharmaceutical Sciences, 2019, 108, 880-887.	1.6	6
62	Glassy behavior of molecular crystals: A comparison between results from MD-simulation and mode coupling theory. Journal of Non-Crystalline Solids, 2006, 352, 4814-4820.	1.5	5
63	Crystallization tendencies of modelled Lennard-Jones liquids with different attractions. Journal of Chemical Physics, 2018, 148, 014501.	1.2	5
64	Structure determination of a new cocrystal of carbamazepine and <scp>DL</scp>-tartaric acid by synchrotron powder X-ray diffraction. Acta Crystallographica Section C, Structural Chemistry, 2020, 76, 225-230.	0.2	5
65	Molecular Dynamics of Generalized Binary Lennard-Jones Systems: Effects of Anharmonicity and Breakdown of the Stokes-Einstein Relation. AIP Conference Proceedings, 2008, , .	0.3	4
66	Influence of pressure on the crystallization of systems characterized by different intermolecular attraction. Physical Review B, 2017, 96, .	1.1	4
67	Molecular Mobility of Terfenadine: Investigation by Dielectric Relaxation Spectroscopy and Molecular Dynamics Simulation. Molecular Pharmaceutics, 2019, 16, 4711-4724.	2.3	4
68	Insight From Molecular Dynamics Simulations on the Crystallization Tendency of Indomethacin Polymorphs in the Undercooled Liquid State. Journal of Pharmaceutical Sciences, 2020, 109, 1086-1095.	1.6	4
69	Structure determination of riboflavin by synchrotron high-resolution powder X-ray diffraction. Acta Crystallographica Section C, Structural Chemistry, 2021, 77, 800-806.	0.2	4
70	Sliding and translational diffusion of molecular phases confined into nanotubes. International Journal of Nanotechnology, 2008, 5, 867.	0.1	3
71	Impact of Amorphization Methods on the Physicochemical Properties of Amorphous Lactulose. Molecular Pharmaceutics, 2020, 17, 1-9.	2.3	3
72	Impact of Low Concentration of Strongly Hydrogen-Bonded Water Molecules on the Dynamics of Amorphous Terfenadine: Insights from Molecular Dynamics Simulations and Dielectric Relaxation Spectroscopy. Journal of Physical Chemistry B, 2021, 125, 11292-11307.	1.2	3

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73	A Molecular Dynamics Simulation of the Orientationaly Disordered Phase of Potassium Perchlorate. Journal De Physique, I, 1996, 6, 149-166.	1.2	3
74	The role of the diffusion in the predictions of the classical nucleation theory for quasi-real systems differ in dipole moment value. Scientific Reports, 2022, 12, .	1.6	3
75	A Computer Simulation Study of Short-Range Order in Metastable hcp Phase of Solid Nitrogen. Journal of Low Temperature Physics, 2001, 122, 211-219.	0.6	2
76	Molecular dynamics simulation of norbornene plastic crystal. Journal of Molecular Structure, 2003, 651-653, 217-221.	1.8	2
77	Slow dynamics in glass-forming materials. Molecular Simulation, 2006, 32, 1057-1068.	0.9	2
78	Morphological and Structural Properties of Amorphous Lactulose Studied by Scanning Electron Microscopy, Polarized Neutron Scattering, and Molecular Dynamics Simulations. Molecular Pharmaceutics, 2020, 17, 10-20.	2.3	2
79	A new criterion for glass-forming ability based on both devitrification and solidification processes. Intermetallics, 2021, 136, 107264.	1.8	2
80	Impact of chirality on the amorphous state of conglomerate forming systems: a case study of N-acetyl-Î±-methylbenzylamine. Physical Chemistry Chemical Physics, 2021, 23, 24282-24293.	1.3	2
81	Pressure Dependence of the Crystallization Rate for the S-Enantiomer and a Racemic Mixture of Ibuprofen. Crystal Growth and Design, 2021, 21, 7075-7086.	1.4	2
82	Neutron spin-echo investigation of orientationally disordered crystal chloroadamantane. Physica B: Condensed Matter, 2004, 350, E1087-E1089.	1.3	1
83	Biopreservative Capabilities of Disaccharides on Proteins: A Study by Molecular Dynamics Simulations. AIP Conference Proceedings, 2008, , .	0.3	1
84	Ab initiostructure determination of two anhydrous forms of Î±-lactose by powder X-ray diffraction. Zeitschrift FÃ¼r Kristallographie, Supplement, 2006, 2006, 595-600.	0.5	1
85	Rotational dynamics in orientationally disordered KClO4. Computational Materials Science, 1998, 10, 57-62.	1.4	0
86	Rotational dynamics and velocity segregation in plastic KClO4 : a molecular dynamics simulation. Molecular Physics, 1998, 93, 703-711.	0.8	0
87	Dynamical transition in orientationally disordered crystals. , 1999, , .		0
88	Dynamics of the rotational degrees of freedom in an undercooled crystal of cyanoadamantane. Phase Transitions, 2003, 76, 781-785.	0.6	0
89	Molecular Dynamics simulations and Neutron Spin Echo experiments of difluorotetrachloroethane glassy crystal. AIP Conference Proceedings, 2004, , .	0.3	0
90	Biopreservation and Homogeneity of Sugar/Water Matrices: A Comparative Study by Molecular Modelling. AIP Conference Proceedings, 2006, , .	0.3	0

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91	Role of pre-peaks in glass-forming liquids. , 2013, , .		0
92	Dynamic disorder in the solid state: insights from dielectric relaxation spectroscopies. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e603-e603.	0.0	0
93	Affinity predictions for cocrystal design: computational versus experimental results. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e551-e551.	0.0	0
94	Manipulation of the crystalline and amorphous physical states of pharmaceutical materials: possibilities, limits and challenges. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e598-e598.	0.0	0