

# Yoshinori Tamai

## List of Publications by Year in descending order

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45  
papers

1,333  
citations

430874

18  
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46  
docs citations

46  
times ranked

1124  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Dynamics Study of Polymer-Water Interaction in Hydrogels. 1. Hydrogen-Bond Structure. <i>Macromolecules</i> , 1996, 29, 6750-6760.	4.8	230
2	Molecular Simulation of Permeation of Small Penetrants through Membranes. 1. Diffusion Coefficients. <i>Macromolecules</i> , 1994, 27, 4498-4508.	4.8	201
3	Molecular Dynamics Study of Polymer-Water Interaction in Hydrogels. 2. Hydrogen-Bond Dynamics. <i>Macromolecules</i> , 1996, 29, 6761-6769.	4.8	158
4	Molecular Simulation of Permeation of Small Penetrants through Membranes. 2. Solubilities. <i>Macromolecules</i> , 1995, 28, 2544-2554.	4.8	97
5	Mean-square radius of gyration of oligo- and poly(methyl methacrylate)s in dilute solutions. <i>Macromolecules</i> , 1990, 23, 4067-4075.	4.8	89
6	Molecular Dynamics Study of Water in Hydrogels. <i>Molecular Simulation</i> , 1996, 16, 359-374.	2.0	42
7	Intrinsic viscosity of oligo- and poly(methyl methacrylate)s. <i>Macromolecules</i> , 1991, 24, 1608-1614.	4.8	38
8	Permeation of small penetrants in hydrogels. <i>Fluid Phase Equilibria</i> , 1998, 144, 441-448.	2.5	35
9	Large Thermal Expansivity of Clathrate Hydrates. <i>Journal of Physical Chemistry B</i> , 1997, 101, 6560-6565.	2.6	34
10	Nanoscale molecular cavity in crystalline polymer membranes studied by molecular dynamics simulation. <i>Polymer</i> , 2003, 44, 3279-3289.	3.8	34
11	Thermally Induced Phase Transition of Crystalline Syndiotactic Polystyrene Studied by Molecular Dynamics Simulation. <i>Macromolecular Rapid Communications</i> , 2002, 23, 891-895.	3.9	31
12	Roles of the Ether Oxygen in Hydration of Tetrahydrofuran Studied by IR, NMR, and DFT Calculation Methods. <i>Journal of Physical Chemistry B</i> , 2009, 113, 906-915.	2.6	30
13	Molecular design of polymer membranes using molecular simulation technique. <i>Fluid Phase Equilibria</i> , 1995, 104, 363-374.	2.5	28
14	Determination by <sup>1</sup> H and <sup>13</sup> C NMR of Stereochemical Compositions of Oligo- and Poly(methyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 22	2.7	28
15	Structure and Potential Surface of Liquid Methanol in Low Temperature: Comparison of the Hydrogen Bond Network in Methanol with Water. <i>Journal of Physical Chemistry B</i> , 1998, 102, 899-905.	2.6	25
16	Reorientational dynamics of aromatic molecules clathrated in $\hat{\Gamma}$ form of crystalline syndiotactic polystyrene. <i>Chemical Physics Letters</i> , 2003, 371, 620-625.	2.6	25
17	Effects of polymer chains on structure and dynamics of supercooled water in poly(vinyl alcohol). <i>Physical Review E</i> , 1999, 59, 5647-5654.	2.1	21
18	Dynamic properties of supercooled water in poly(vinyl alcohol) hydrogel. <i>Chemical Physics Letters</i> , 1998, 285, 127-132.	2.6	20

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19	Molecular dynamics study of temperature dependence of volume of amorphous silica. Journal of Non-Crystalline Solids, 2004, 349, 319-330.	3.1	19
20	Reorientational relaxation of aromatic molecules in the molecular cavity of crystalline syndiotactic polystyrene studied by molecular dynamics simulation. Journal of Molecular Structure, 2005, 739, 33-40.	3.6	19
21	Effect of encaged aromatic guests on the shape and connectivity of molecular cavity in crystalline polystyrene evaluated by molecular simulations. Journal of Chemical Physics, 2004, 121, 12085-12093.	3.0	17
22	Structure and Dynamics of Poly(Vinyl Alcohol) Hydrogel. Molecular Simulation, 1999, 21, 283-301.	2.0	12
23	Fast one-dimensional gas transport in molecular capillary embedded in polymer crystal. Chemical Physics Letters, 2003, 371, 217-222.	2.6	12
24	Rearrangement of Nanoporous Cavity Structures in Crystalline Syndiotactic Polystyrene Associated with Stress-Induced Phase Transition. ACS Macro Letters, 2013, 2, 834-838.	4.8	11
25	Formation of a 6FDA-based ring polyimide with nanoscale cavity evaluated by DFT calculations. Journal of Molecular Structure, 2005, 739, 105-115.	3.6	9
26	Sorption of organic solvents on the surface of crystalline syndiotactic polystyrene studied by molecular dynamics simulation. Journal of Molecular Structure, 2005, 739, 27-32.	3.6	8
27	Structural change in the process of permanent densification of fluorozirconate glass studied with molecular dynamics simulations. Physical Review B, 2000, 62, 865-873.	3.2	7
28	Role of structural relaxation in peculiar permanent densification of fluorozirconate glass. Journal of Chemical Physics, 2000, 112, 3875-3883.	3.0	7
29	Molecular dynamics simulation of permanent densification of fluorozirconate glass. Chemical Physics Letters, 1999, 302, 15-19.	2.6	6
30	Structural Analysis of Molecular Cavity Using a 3D Printer. Journal of Computer Chemistry Japan, 2016, 15, 97-104.	0.1	6
31	Diffusion mechanism of CO <sub>2</sub> in a crystalline polymer membrane studied using model gases. Molecular Simulation, 2015, 41, 974-979.	2.0	5
32	A practical method to determine glass transition temperature in molecular dynamics simulation of mixed ionic glasses. Chemical Physics Letters, 2002, 351, 99-104.	2.6	4
33	Molecular dynamics simulations of structural transitions of crystalline polystyrene in response to external stresses and temperatures. Polymer, 2017, 128, 177-187.	3.8	4
34	Molecular dynamics simulation of high-pressure densification of fluorozirconate glass. Journal of Non-Crystalline Solids, 2002, 306, 282-291.	3.1	3
35	Effects of pressure on the fragile nature of fluorozirconates studied by molecular dynamics simulations. Physical Review E, 2003, 67, 031504.	2.1	3
36	Molecular Dynamics Study of Compressibility of Vitreous Silica. Japanese Journal of Applied Physics, 2005, 44, 8086-8087.	1.5	3

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37	Effective and efficient transport mechanism of CO <sub>2</sub> in subnano-porous crystalline membrane of syndiotactic polystyrene. <i>Journal of Membrane Science</i> , 2022, 646, 120202.	8.2	3
38	Molecular Dynamics Simulation of Polymers-Interaction between Polymer and Small Molecules-. <i>Kobunshi</i> , 2004, 53, 258-262.	0.0	2
39	Molecular Dynamics Study of Fictive Temperature Dependence of Density of Vitreous Silica. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 7550-7551.	1.5	2
40	Construction of Layered Structure of Rigid-Rod Polyesters with Flexible Side Chains by a Molecular Dynamics Simulation. <i>Journal of Computer Chemistry Japan</i> , 2004, 3, 13-20.	0.1	2
41	Molecular Dynamic Study on Structure of Interface Formed by Binding Flat Amorphous Silica Surfaces at High Temperatures. <i>Japanese Journal of Applied Physics</i> , 2005, 44, 7539-7545.	1.5	1
42	Guest Occupation Effects on the Transition of Crystalline Syndiotactic Polystyrene: Selection Criteria for Fundamental Structures $\beta$ and $\beta'$ . <i>Macromolecular Theory and Simulations</i> , 2018, 27, 1.4 1800039.		1
43	Sorption Mechanism of Aromatic Molecules in the Interface between Liquid and Polymer Crystal. <i>Molecular Simulation</i> , 2004, 30, 901-906.	2.0	0
44	Solubility of Noble and Hydrocarbon Gases in Poly(dimethylsiloxane) Using Test-Particle-Insertion Method. <i>Kobunshi Ronbunshu</i> , 2010, 67, 203-208.	0.2	0
45	Computer Simulation in Polymer Physical Chemistry and Its Application to Biomolecules. <i>Seibutsu Butsuri</i> , 2007, 47, 390-396.	0.1	0