Shinichi Miura

List of Publications by Year
in descending order

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53	943	623734	454955
papers	citations	14 h-index	30 g-index

53	53	53	610
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	An Efficient Replica Exchange Monte Carlo Method Using the Gaussian Ensemble for First-Order Transitions. Journal of the Physical Society of Japan, 2022, 91, .	1.6	1
2	Potential energy landscape and thermodynamic transitions of coarse-grained protein models revealed by the multicanonical generalized hybrid Monte Carlo method. Biophysics and Physicobiology, 2020, 17, 14-24.	1.0	1
3	Molecular dynamics study on fast diffusion of hydrogen molecules in filled ice II. Journal of Molecular Liquids, 2019, 292, 111316.	4.9	3
4	Quantum structural fluctuations of protonated water clusters (H2O) H+ (nâ€¯=â€¯1â€¯â^'â€¯4) studied by variational molecular dynamics method. Journal of Molecular Liquids, 2019, 284, 157-162.	4.9	0
5	Quantum structural fluctuation in para-hydrogen clusters revealed by the variational path integral method. Journal of Chemical Physics, 2018, 148, 102333.	3.0	5
6	Development of a generalized hybrid Monte Carlo algorithm to generate the multicanonical ensemble with applications to molecular systems. Journal of Chemical Physics, 2018, 149, 072322.	3.0	3
7	Comparative study of 3D-RISM theory and molecular dynamics calculations for the free-energy landscape of a hydrated dipeptide. Molecular Simulation, 2017, 43, 1406-1411.	2.0	2
8	On computational efficiency of the hybrid Monte Carlo method applied to the multicanonical ensemble. Molecular Simulation, 2017, 43, 1291-1294.	2.0	2
9	Variational path integral molecular dynamics and hybrid Monte Carlo algorithms using a fourth order propagator with applications to molecular systems. Journal of Chemical Physics, 2016, 145, 074114.	3.0	12
10	Quantum Structural Fluctuation in Molecular Hydrogen Clusters. Journal of Computer Chemistry Japan, 2016, 15, 136-142.	0.1	1
11	Isotope effects of ammonia umbrella flip using semiclassical instanton calculations based on discretized path integrals. Chemical Physics Letters, 2015, 634, 146-150.	2.6	5
12	The isotope effects on a hydrogen transfer using path integral instanton method. Molecular Simulation, 2015, 41, 861-867.	2.0	0
13	Analytical expressions on harmonic oscillators for variational path integrals. Molecular Simulation, 2015, 41, 808-812.	2.0	3
14	A 3D-RISM integral equation study of a hydrated dipeptide. Molecular Simulation, 2015, 41, 1015-1020.	2.0	3
15	Efficient algorithms for semiclassical instanton calculations based on discretized path integrals. Journal of Chemical Physics, 2014, 141, 024101.	3.0	14
16	Variational path integral molecular dynamics study of a water molecule. Journal of Physics: Conference Series, 2013, 454, 012023.	0.4	5
17	An efficient computational method for the implementation of a semi-classical instanton approach using discretized path integrals. Journal of Physics: Conference Series, 2013, 454, 012030.	0.4	3
18	A variational path integral molecular dynamics method applied to molecular vibrational fluctuations. Molecular Simulation, 2012, 38, 378-383.	2.0	8

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19	Molecular Dynamics and Hybrid Monte Carlo Algorithms for the Variational Path Integral with a Fourth-Order Propagator. ACS Symposium Series, 2012, , 177-186.	0.5	3
20	First-principles study of spontaneous polarisation and water dipole moment in ferroelectric ice XI. Molecular Simulation, 2012, 38, 369-372.	2.0	4
21	Variational Path Integral Molecular Dynamics Study of Small Para-Hydrogen Clusters. Progress in Theoretical Chemistry and Physics, 2012, , 427-436.	0.2	1
22	A variational path integral molecular dynamics study of a solid helium-4. Computer Physics Communications, 2011, 182, 274-276.	7.5	13
23	Molecular dynamics algorithms for quantum Monte Carlo methods. Chemical Physics Letters, 2009, 482, 165-170.	2.6	14
24	Quantum rotational fluctuation of a linear molecule doped in superfluid helium clusters. Journal of Physics Condensed Matter, 2008, 20, 494205.	1.8	3
25	Quantum Fluctuations of an OCS Molecule in Superfluid Helium-4 Clusters. AIP Conference Proceedings, 2008, , .	0.4	0
26	Rotational fluctuation of molecules in quantum clusters. I. Path integral hybrid Monte Carlo algorithm. Journal of Chemical Physics, 2007, 126, 114308.	3.0	21
27	Rotational fluctuation of molecules in quantum clusters. II. Molecular rotation and superfluidity in OCS-doped helium-4 clusters. Journal of Chemical Physics, 2007, 126, 114309.	3.0	26
28	Path Integral Hybrid Monte Carlo Study on Structure of Small Helium-4 Clusters Doped with a Linear Molecule. Journal of Low Temperature Physics, 2007, 148, 839-843.	1.4	3
29	On the solvation structure of a raregas solute in superfluid helium-4. Journal of Molecular Liquids, 2005, 119, 41-46.	4.9	1
30	Quantum rotation of carbonyl sulfide molecules in superfluid helium clusters: a path integral hybrid Monte Carlo study. Journal of Physics Condensed Matter, 2005, 17, S3259-S3264.	1.8	10
31	Path integral hybrid Monte Carlo algorithm for correlated Bose fluids. Journal of Chemical Physics, 2004, 120, 2160-2168.	3.0	28
32	A large-scale molecular dynamics study of dynamic structure factor and dispersion relation of acoustic mode in liquid and supercritical water. Fluid Phase Equilibria, 2004, 226, 345-350.	2.5	13
33	A unified scheme forab initiomolecular orbital theory and path integral molecular dynamics. Journal of Chemical Physics, 2001, 115, 9149-9159.	3.0	126
34	A generalized Ornsteinâ€“Zernike integral equation study of atomic impurities in quantum fluids. Journal of Chemical Physics, 2001, 115, 4161-4168.	3.0	10
35	A molecular approach to quantum fluids based on a generalized Ornsteinâ€“Zernike integral equation. Journal of Chemical Physics, 2001, 114, 7497-7505.	3.0	10
36	Path integral hybrid Monte Carlo calculation of the bosonic oscillators. Journal of Molecular Liquids, 2001, 90, 21-28.	4.9	0

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37	Density matrix and eigenstates for an excess electron in water. Journal of Molecular Liquids, 2001, 90, 225-231.	4.9	3
38	A molecular dynamics study of dielectric constant of water from ambient to sub- and supercritical conditions using a fluctuating-charge potential model. Chemical Physics Letters, 2001, 345, 195-200.	2.6	69
39	Isotope effect on the structure of quantum fluid: a generalized Ornsteinâ€“Zernike analysis. Chemical Physics Letters, 2001, 337, 306-312.	2.6	1
40	Path integral molecular dynamics method based on a pair density matrix approximation: An algorithm for distinguishable and identical particle systems. Journal of Chemical Physics, 2001, 115, 5353-5361.	3.0	7
41	Ab initio molecular orbital calculation considering the quantum mechanical effect of nuclei by path integral molecular dynamics. Chemical Physics Letters, 2000, 332, 396-402.	2.6	84
42	A molecular-dynamics study of the equation of state of water using a fluctuating-charge model. Chemical Physics Letters, 2000, 317, 414-420.	2.6	25
43	Path integral molecular dynamics for Boseâ€“Einstein and Fermiâ€“Dirac statistics. Journal of Chemical Physics, 2000, 112, 10116-10124.	3.0	32
44	Path integral hybrid Monte Carlo for the bosonic many-body systems. Chemical Physics Letters, 1999, 308, 115-122.	2.6	6
45	A path integral centroid molecular dynamics study of nonsuperfluid liquid helium-4. Journal of Chemical Physics, 1999, 110, 4523-4532.	3.0	55
46	Density Fluctuation and Hydrogen-Bonded Clusters in Supercritical Water. A Molecular Dynamics Analysis Using a Polarizable Potential Model. Bulletin of the Chemical Society of Japan, 1999, 72, 151-162.	3.2	22
47	A molecular dynamics study of sub- and supercritical water using a polarizable potential model. Journal of Chemical Physics, 1998, 109, 4873-4884.	3.0	101
48	An ab initio path integral molecular dynamics study of double proton transfer in the formic acid dimer. Journal of Chemical Physics, 1998, 109, 5290-5299.	3.0	107
49	A Molecular Dynamics Study of P .RHO. T-Diagram of Sub- and Supercritical Water Using a Polarizable Potential Model.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 1998, 7, 1115-1117.	0.0	6
50	Anomalous acoustic dynamics in liquid water: the origin of the low frequency mode. Molecular Physics, 1996, 87, 1405-1421.	1.7	7
51	Anomalous acoustic dynamics in liquid water: the origin of the low frequency mode. Molecular Physics, 1996, 87, 1405-1421.	1.7	2
52	Molecular Theory for the Nonequilibrium Free Energy Profile in Electron Transfer Reaction. The Journal of Physical Chemistry, 1995, 99, 10526-10529.	2.9	39
53	Temperature Dependence of the Stability of a Hydrated Electron: An Integral Equation Study. The Journal of Physical Chemistry, 1994, 98, 9649-9656.	2.9	20