# 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 | A unified scheme forab initiomolecular orbital theory and path integral molecular dynamics. Journal of Chemical Physics, 2001, 115, 9149-9159. | 3.0 | 126 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | A path integral centroid molecular dynamics study of nonsuperfluid liquid helium-4. Journal of Chemical Physics, 1999, 110, 4523-4532. | 3.0 | 55 |
| 7 | Molecular Theory for the Nonequilibrium Free Energy Profile in Electron Transfer Reaction. The Journal of Physical Chemistry, 1995, 99, 10526-10529. | 2.9 | 39 |
| 8 | Path integral molecular dynamics for Boseâ€“Einstein and Fermiâ€“Dirac statistics. Journal of Chemical Physics, 2000, 112, 10116-10124. | 3.0 | 32 |
| 9 | Path integral hybrid Monte Carlo algorithm for correlated Bose fluids. Journal of Chemical Physics, 2004, 120, 2160-2168. | 3.0 | 28 |
| 10 | 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 |
| 11 | 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 |
| 12 | 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 |
| 13 | Rotational fluctuation of molecules in quantum clusters. I. Path integral hybrid Monte Carlo algorithm. Journal of Chemical Physics, 2007, 126, 114308. | 3.0 | 21 |
| 14 | 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 |
| 15 | Molecular dynamics algorithms for quantum Monte Carlo methods. Chemical Physics Letters, 2009, 482, 165-170. | 2.6 | 14 |
| 16 | Efficient algorithms for semiclassical instanton calculations based on discretized path integrals. Journal of Chemical Physics, 2014, 141, 024101. | 3.0 | 14 |
| 17 | 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 |
| 18 | A variational path integral molecular dynamics study of a solid helium-4. Computer Physics Communications, 2011, 182, 274-276. | 7.5 | 13 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | A generalized Ornsteinâ€“Zernike integral equation study of atomic impurities in quantum fluids. Journal of Chemical Physics, 2001, 115, 4161-4168. | 3.0 | 10 |
| 21 | 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 |
| 22 | 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 |
| 23 | A variational path integral molecular dynamics method applied to molecular vibrational fluctuations. Molecular Simulation, 2012, 38, 378-383. | 2.0 | 8 |
| 24 | Anomalous acoustic dynamics in liquid water: the origin of the low frequency mode. Molecular Physics, 1996, 87, 1405-1421. | 1.7 | 7 |
| 25 | 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 |
| 26 | 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 |
| 27 | Path integral hybrid Monte Carlo for the bosonic many-body systems. Chemical Physics Letters, 1999, 308, 115-122. | 2.6 | 6 |
| 28 | Variational path integral molecular dynamics study of a water molecule. Journal of Physics: Conference Series, 2013, 454, 012023. | 0.4 | 5 |
| 29 | 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 |
| 30 | Quantum structural fluctuation in para-hydrogen clusters revealed by the variational path integral method. Journal of Chemical Physics, 2018, 148, 102333. | 3.0 | 5 |
| 31 | First-principles study of spontaneous polarisation and water dipole moment in ferroelectric ice XI. Molecular Simulation, 2012, 38, 369-372. | 2.0 | 4 |
| 32 | Density matrix and eigenstates for an excess electron in water. Journal of Molecular Liquids, 2001, 90, 225-231. | 4.9 | 3 |
| 33 | 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 |
| 34 | Quantum rotational fluctuation of a linear molecule doped in superfluid helium clusters. Journal of Physics Condensed Matter, 2008, 20, 494205. | 1.8 | 3 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | Analytical expressions on harmonic oscillators for variational path integrals. Molecular Simulation, 2015, 41, 808-812. | 2.0 | 3 |
| 38 | A 3D-RISM integral equation study of a hydrated dipeptide. Molecular Simulation, 2015, 41, 1015-1020. | 2.0 | 3 |
| 39 | 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 |
| 40 | Molecular dynamics study on fast diffusion of hydrogen molecules in filled ice II. Journal of Molecular Liquids, 2019, 292, 111316. | 4.9 | 3 |
| 41 | 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 |
| 42 | On computational efficiency of the hybrid Monte Carlo method applied to the multicanonical ensemble. Molecular Simulation, 2017, 43, 1291-1294. | 2.0 | 2 |
| 43 | Anomalous acoustic dynamics in liquid water: the origin of the low frequency mode. Molecular Physics, 1996, 87, 1405-1421. | 1.7 | 2 |
| 44 | Isotope effect on the structure of quantum fluid: a generalized Ornsteinâ€“Zernike analysis. Chemical Physics Letters, 2001, 337, 306-312. | 2.6 | 1 |
| 45 | On the solvation structure of a raregas solute in superfluid helium-4. Journal of Molecular Liquids, 2005, 119, 41-46. | 4.9 | 1 |
| 46 | 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 |
| 47 | Variational Path Integral Molecular Dynamics Study of Small Para-Hydrogen Clusters. Progress in Theoretical Chemistry and Physics, 2012, , 427-436. | 0.2 | 1 |
| 48 | Quantum Structural Fluctuation in Molecular Hydrogen Clusters. Journal of Computer Chemistry Japan, 2016, 15, 136-142. | 0.1 | 1 |
| 49 | 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 |
| 50 | Path integral hybrid Monte Carlo calculation of the bosonic oscillators. Journal of Molecular Liquids, 2001, 90, 21-28. | 4.9 | 0 |
| 51 | Quantum Fluctuations of an OCS Molecule in Superfluid Helium-4 Clusters. AIP Conference Proceedings, 2008, , . | 0.4 | 0 |
| 52 | The isotope effects on a hydrogen transfer using path integral instanton method. Molecular Simulation, 2015, 41, 861-867. | 2.0 | 0 |
| 53 | Quantum structural fluctuations of protonated water clusters (H2O) H+ (nâ€¯=â€¯1â€¯â^¼â€¯4) studied by variational molecular dynamics method. Journal of Molecular Liquids, 2019, 284, 157-162. | 4.9 | 0 |