Igor P Omelyan

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8678553/publications.pdf

Version: 2024-02-01

59	1,087	567281 15	434195 31
papers	citations	h-index	g-index

59	59	59	678
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations. Computer Physics Communications, 2003, 151, 272-314.	7.5	180
2	Generalized collective modes for the Lennard-Jones fluid. Molecular Physics, 1995, 84, 235-259.	1.7	101
3	On the numerical integration of motion for rigid polyatomics: The modified quaternion approach. Computers in Physics, 1998, 12, 97.	0.5	67
4	Optimized Forestâ€“Ruth- and Suzuki-like algorithms for integration of motion in many-body systems. Computer Physics Communications, 2002, 146, 188-202.	7.5	67
5	Algorithm for Molecular Dynamics Simulations of Spin Liquids. Physical Review Letters, 2001, 86, 898-901.	7.8	66
6	Algorithm for numerical integration of the rigid-body equations of motion. Physical Review E, 1998, 58, 1169-1172.	2.1	53
7	Compressibility oftert-Butyl Alcohol-Water Mixtures: The Rism Theory. Journal of Theoretical and Computational Chemistry, 2003, 02, 193-203.	1.8	37
8	MTS-MD of Biomolecules Steered with 3D-RISM-KH Mean Solvation Forces Accelerated with Generalized Solvation Force Extrapolation. Journal of Chemical Theory and Computation, 2015, 11, 1875-1895.	5.3	36
9	Generalized collective modes for a Lennard-Jones fluid in higher-mode approximations. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 205, 401-406.	2.1	26
10	Ferromagnetic Phase Transition in a Heisenberg Fluid: Monte Carlo Simulations and Fisher Corrections to Scaling. Physical Review Letters, 2001, 86, 3156-3159.	7.8	25
11	Numerical integration of the equations of motion for rigid polyatomics: The matrix method. Computer Physics Communications, 1998, 109, 171-183.	7.5	24
12	Longitudinal wavevector- and frequency-dependent dielectric constant of the TIP4P water model. Molecular Physics, 1998, 93, 123-135.	1.7	21
13	Multiple time step molecular dynamics in the optimized isokinetic ensemble steered with the molecular theory of solvation: Accelerating with advanced extrapolation of effective solvation forces. Journal of Chemical Physics, 2013, 139, 244106.	3.0	20
14	Generalised canonicalâ€“isokinetic ensemble: speeding up multiscale molecular dynamics and coupling with 3D molecular theory of solvation. Molecular Simulation, 2013, 39, 25-48.	2.0	17
15	Advanced gradientlike methods for rigid-body molecular dynamics. Journal of Chemical Physics, 2007, 127, 044102.	3.0	15
16	On the reaction field for interaction site models of polar systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 223, 295-302.	2.1	14
17	A New Leapfrog Integrator of Rotational Motion. The Revised Angular-Momentum Approach. Molecular Simulation, 1999, 22, 213-236.	2.0	14
18	Ewald summation technique for interaction site models of polar fluids. Computer Physics Communications, 1997, 107, 113-122.	7.5	13

#	Article	IF	Citations
19	Cavity formation energies for diatomic and spherical solutes in a diatomic hard body fluid. Journal of Chemical Physics, 2000, 113, 4349-4358.	3.0	13
20	Microscopic description of a liquidâ€“vapor interface by an inhomogeneous integral equation theory. Chemical Physics Letters, 2004, 397, 368-373.	2.6	13
21	Criticality of a liquidâ€“vapor interface from an inhomogeneous integral equation theory. Physical Chemistry Chemical Physics, 2005, 7, 4132.	2.8	13
22	Generalized dipolar modes of a Stockmayer fluid in high-order approximations. Physical Review E, 1998, 57, 6667-6676.	2.1	12
23	Efficient algorithms for rigid body integration using optimized splitting methods and exact free rotational motion. Journal of Chemical Physics, 2008, 128, 136102.	3.0	12
24	Processed splitting algorithms for rigid-body molecular dynamics simulations. Physical Review E, 2008, 78, 026702.	2.1	12
25	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. II. Canonical and isokinetic ensembles. Journal of Chemical Physics, 2011, 135, 234107.	3.0	12
26	Overcoming the Barrier on Time Step Size in Multiscale Molecular Dynamics Simulation of Molecular Liquids. Journal of Chemical Theory and Computation, 2012, 8, 6-16.	5.3	12
27	Generalized mode approach 3. Generalized transport coefficients of a Lennard-Jones fluid. Molecular Physics, 1997, 92, 913-928.	1.7	12
28	Kinetic equation for liquids with a multistep potential of interaction. H-theorem. Physica A: Statistical Mechanics and Its Applications, 1996, 234, 89-107.	2.6	11
29	The influence of molecular shape on chemical reaction thermodynamics. Journal of Chemical Physics, 2001, 115, 9401-9409.	3.0	11
30	Wavevector- and frequency-dependent dielectric constant of the Stockmayer fluid. Molecular Physics, 1996, 87, 1273-1283.	1.7	10
31	Improved cubature formulae of high degrees of exactness for the square. Journal of Computational and Applied Mathematics, 2006, 188, 190-204.	2.0	10
32	Consistent Description of Kinetics and Hydrodynamics of Weakly Nonequilibrium Processes in Simple Liquids. Journal of Statistical Physics, 2014, 155, 843-866.	1.2	10
33	Spatially inhomogeneous population dynamics: beyond the mean field approximation. Journal of Physics A: Mathematical and Theoretical, 2019, 52, 305601.	2.1	10
34	Advanced multiple time scale molecular dynamics. Journal of Chemical Physics, 2009, 131, 104101.	3.0	9
35	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. I. Microcanonical ensemble. Journal of Chemical Physics, 2011, 135, 114110.	3.0	9
36	Kinetic equation for liquids with a multistep potential of interaction: Calculation of transport coefficients. Physical Review E, 2000, 62, 8021-8036.	2.1	7

#	Article	IF	Citations
37	The modified collective-mode approach: dielectric relaxation in water. Journal of Physics Condensed Matter, 2000, 12, L505-L512.	1.8	7
38	Self-consistent corrections to the equation of state and chemical potentials of hard chain fluid mixtures. Journal of Chemical Physics, 2001, 114, 5735-5744.	3.0	7
39	Interpretation of atomic motion in flexible molecules: Accelerating molecular dynamics simulations. Physical Review E, 2012, 85, 026706.	2.1	7
40	On the calculation of temperature derivatives for the dielectric constant in computer simulations. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 208, 237-243.	2.1	6
41	Generalized collective mode approach in the dielectric theory of dipolar systems. Physica A: Statistical Mechanics and Its Applications, 1997, 247, 121-139.	2.6	6
42	Nonequilibrium statistical operator in the generalized molecular hydrodynamics of fluids. Theoretical and Mathematical Physics(Russian Federation), 2008, 154, 75-84.	0.9	6
43	Relaxation to the state of molecular hydrodynamics in the generalized hydrodynamics of liquids. Physical Review E, 2010, 82, 041202.	2.1	6
44	Wavevector dependent dielectric constant of the MCY water model. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 220, 167-177.	2.1	5
45	Liquid-vapor and liquid-liquid interfaces in Ising fluids: An integral equation approach. Journal of Chemical Physics, 2007, 126, 124702.	3.0	5
46	Enhanced solvation force extrapolation for speeding up molecular dynamics simulations of complex biochemical liquids. Journal of Chemical Physics, 2019, 151, 214102.	3.0	5
47	Spatial population dynamics: Beyond the Kirkwood superposition approximation by advancing to the Fisherâ€“Kopeliovich ansatz. Physica A: Statistical Mechanics and Its Applications, 2020, 544, 123546.	2.6	5
48	Temperature behavior of the frequency-dependent dielectric constant for a Stockmayer fluid. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 216, 211-216.	2.1	4
49	Transverse wavevector dependent and frequency dependent dielectric function, magnetic permittivity and generalized conductivity of interaction site fluids: MD calculations for the TIP4P water. Molecular Physics, 1999, 96, 407-427.	1.7	4
50	Conservation-laws-preserving algorithms for spin dynamics simulations. Europhysics Letters, 2000, 52, 603-609.	2.0	4
51	Generalized mode approach 2. Longitudinal time correlation functions of a Lennard-Jones fluid. Molecular Physics, 1997, 91, 1005-1015.	1.7	4
52	On the derivation of the dipole moment fluctuation formulas for finite systems. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 212, 279-284.	2.1	2
53	Normal solution and transport coefficients to the Enskogâ€“Landau kinetic equation for a two-component system of charged hard spheres: The Chapmanâ€“Enskog method. Physica A: Statistical Mechanics and Its Applications, 1999, 268, 607-628.	2.6	2
54	Chemical potentials of chain solutes in hard body fluids. Journal of Molecular Liquids, 2001, 92, 3-14.	4.9	2

#	Article	IF	Citations
55	Transverse wavevector dependent and frequency dependent dielectric function, magnetic permittivity and generalized conductivity of interaction site fluids: MD calculations for the TIP4P water. Molecular Physics, 1999, 96, 407-427.	1.7	2
56	Normal solution to the Enskog-Landau kinetic equation: boundary conditions method. Physics Letters, Section A: General, Atomic and Solid State Physics, 1996, 223, 37-44.	2.1	1
57	Jumps and coalescence in the continuum: A numerical study. Applied Mathematics and Computation, 2021, 390, 125610.	2.2	1
58	Algorithm for numerical solutions to the kinetic equation of a spatial population dynamics model with coalescence and repulsive jumps. Numerical Algorithms, 2021, 87, 895-919.	1.9	1
59	Wavevector- and frequency-dependent dielectric constant of the Stockmayer fluid. Molecular Physics, 1996, 87, 1273-1283.	1.7	1