

Gennady Chuev

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6514992/publications.pdf>

Version: 2024-02-01

59
papers

1,255
citations

471509

17
h-index

377865

34
g-index

60
all docs

60
docs citations

60
times ranked

1132
citing authors

#	ARTICLE	IF	CITATIONS
1	NWChem: Past, present, and future. <i>Journal of Chemical Physics</i> , 2020, 152, 184102.	3.0	425
2	Improved estimates for hydration free energy obtained by the reference interaction site model. <i>Chemical Physics Letters</i> , 2007, 448, 198-202.	2.6	94
3	An Accurate Prediction of Hydration Free Energies by Combination of Molecular Integral Equations Theory with Structural Descriptors. <i>Journal of Physical Chemistry B</i> , 2010, 114, 12068-12079.	2.6	74
4	Wavelet algorithm for solving integral equations of molecular liquids. A test for the reference interaction site model. <i>Journal of Computational Chemistry</i> , 2004, 25, 1369-1377.	3.3	45
5	An operational Haar wavelet method for solving fractional Volterra integral equations. <i>International Journal of Applied Mathematics and Computer Science</i> , 2011, 21, 535-547.	1.5	39
6	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. <i>Journal of Computational Chemistry</i> , 2008, 29, 2406-2415.	3.3	38
7	Integral Equation Theory of Molecular Solvation Coupled with Quantum Mechanical/Molecular Mechanics Method in NWChem Package. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1246-1254.	5.3	31
8	Wavelet treatment of structure and thermodynamics of simple liquids. <i>Journal of Chemical Physics</i> , 2004, 120, 1191-1196.	3.0	29
9	Reference interaction site model study of self-aggregating cyanine dyes. <i>Journal of Chemical Physics</i> , 2009, 131, 074503.	3.0	29
10	Hydration structure of osmolyte TMAO: concentration/pressure-induced response. <i>New Journal of Chemistry</i> , 2017, 41, 1219-1228.	2.8	28
11	Hydration of Hydrophobic Solutes Treated by the Fundamental Measure Approach. <i>Journal of Physical Chemistry B</i> , 2006, 110, 18496-18503.	2.6	25
12	A structured low-rank wavelet solver for the Ornstein-Zernike integral equation. <i>Computing (Vienna/New York)</i> , 2007, 80, 47-73.	4.8	21
13	Comparative study of electrostatic solvent response by RISM and PCM methods. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 265-274.	2.0	20
14	In Silico Screening of Bioactive and Biomimetic Solutes Using Molecular Integral Equation Theory. <i>Current Pharmaceutical Design</i> , 2011, 17, 1695-1708.	1.9	20
15	Features of local ordering of biocompatible ionic liquids: The case of choline-based amino acid ionic liquids. <i>Journal of Molecular Liquids</i> , 2019, 296, 112081.	4.9	20
16	Local ion hydration structure in aqueous imidazolium-based ionic liquids: The effects of concentration and anion nature. <i>Journal of Molecular Liquids</i> , 2017, 247, 100-108.	4.9	19
17	Extraction of atom-atom bridge and direct correlation functions from molecular simulations: A test for ambient water. <i>Chemical Physics Letters</i> , 2013, 561-562, 175-178.	2.6	18
18	Hydration features of the neurotransmitter acetylcholine. <i>Journal of Molecular Liquids</i> , 2020, 304, 112757.	4.9	17

#	ARTICLE	IF	CITATIONS
19	Wavelet treatment of radial distribution functions of solutes. <i>Physical Review E</i> , 2003, 68, 027702.	2.1	16
20	Density functional method based on wavelets for quantum classical systems. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 539-547.	2.0	14
21	Nature of the metal–nonmetal transition in metal–ammonia solutions. I. Solvated electrons at low metal concentrations. <i>Journal of Chemical Physics</i> , 2007, 127, 244501.	3.0	14
22	A Polaron Model for Electron Transfer in Globular Proteins. <i>Journal of Theoretical Biology</i> , 1993, 163, 51-60.	1.7	13
23	Density functional study of polarons and bipolarons in polar liquids. <i>Physical Review B</i> , 2003, 67, .	3.2	13
24	Wavelet method for solving integral equations of simple liquids. <i>Journal of Molecular Liquids</i> , 2005, 120, 159-162.	4.9	13
25	3D WAVELET TREATMENT OF SOLVATED BIPOLARON AND POLARON. <i>Journal of Theoretical and Computational Chemistry</i> , 2005, 04, 751-767.	1.8	12
26	Nature of metal–nonmetal transition in metal–ammonia solutions. II. From uniform metallic state to inhomogeneous electronic microstructure. <i>Journal of Chemical Physics</i> , 2008, 128, 144503.	3.0	12
27	Extraction of site–site bridge functions and effective pair potentials from simulations of polar molecular liquids. <i>Journal of Computational Chemistry</i> , 2014, 35, 1010-1023.	3.3	12
28	Site density models of inhomogeneous classical molecular liquids. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2018, 2018, 093201.	2.3	12
29	Mean-field theory of an electron solvated in molten salts. <i>Journal of Chemical Physics</i> , 2000, 112, 4707-4715.	3.0	11
30	Triangular functions for operational matrix of nonlinear fractional Volterra integral equations. <i>Journal of Applied Mathematics and Computing</i> , 2015, 49, 213-232.	2.5	11
31	Chemical bond effects in classical site density functional theory of inhomogeneous molecular liquids. <i>Journal of Chemical Physics</i> , 2020, 152, 041101.	3.0	10
32	Density functional theory of bipolarons in polar liquids. <i>Chemical Physics Letters</i> , 2003, 368, 53-58.	2.6	9
33	Superexchange coupling and electron transfer in globular proteins via polaron excitations. <i>Journal of Biological Physics</i> , 2000, 26, 173-184.	1.5	8
34	Mean-field treatment of polarons in strong electrolytes. <i>Physical Review E</i> , 2001, 63, 061204.	2.1	8
35	Wavelet treatment of the intrachain correlation functions of homopolymers in dilute solutions. <i>Physical Review E</i> , 2004, 70, 051803.	2.1	8
36	Molecular insight on ion hydration and association in aqueous choline chloride solutions. <i>Journal of Molecular Liquids</i> , 2020, 313, 113563.	4.9	8

#	ARTICLE	IF	CITATIONS
37	Herzfeld instability versus Mott transition in metal-ammonia solutions. <i>Comptes Rendus Physique</i> , 2007, 8, 449-455.	0.9	7
38	Renormalized site density functional theory. <i>Journal of Statistical Mechanics: Theory and Experiment</i> , 2021, 2021, 033205.	2.3	7
39	Renormalized site density functional theory for models of ion hydration. <i>Journal of Chemical Physics</i> , 2021, 155, 064501.	3.0	6
40	CDFTPY: A python package for performing classical density functional theory calculations for molecular liquids. <i>Computer Physics Communications</i> , 2022, 276, 108338.	7.5	6
41	Statistical theory of a solvated electron in an electrolyte. <i>Journal of Experimental and Theoretical Physics</i> , 1999, 88, 807-814.	0.9	5
42	Bipolarons in a KCl melt. <i>Journal of Experimental and Theoretical Physics</i> , 2000, 91, 983-990.	0.9	5
43	Comment on "Model of saturated lithium ammonia as a single-component liquid metal". <i>J. Chem. Phys.</i> 124, 074702 (2006). <i>Journal of Chemical Physics</i> , 2008, 128, 027101.	3.0	5
44	Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. <i>Molecules</i> , 2022, 27, 799.	3.8	5
45	Quantum mechanics of solvated complexes: A test for positronium. <i>International Journal of Quantum Chemistry</i> , 2002, 88, 634-641.	2.0	4
46	Dispersion forces between solvated electrons. <i>Journal of Chemical Physics</i> , 2010, 132, 144504.	3.0	2
47	Non-metal-to-metal transition driven by van der Waals forces in an interacting polaronic gas. <i>New Journal of Physics</i> , 2010, 12, 023030.	2.9	2
48	Superexchange coupling and electron transfer in globular proteins via polaron excitations. <i>Journal of Biological Physics</i> , 1999, 24, 245-256.	1.5	1
49	A probabilistic method for calculating the energy of hydrophobic interactions. <i>Biophysics (Russian)</i> Tj ETQq1 1 0.784314 rgBT ₁ /Overlo	0.7	1
50	Electron-electron attraction caused by dispersion forces in metal-ammonia solutions. <i>Chemical Physics Letters</i> , 2013, 556, 138-141.	2.6	1
51	Exact site-site bridge functions for dielectric consistent reference interaction site model: A test for ambient water. <i>Journal of Molecular Liquids</i> , 2015, 205, 67-73.	4.9	1
52	Hybrid Functions of Lagrange Polynomials and Block-Pulse Functions for Solving Integro-partial Differential Equations. <i>Iranian Journal of Science and Technology, Transaction A: Science</i> , 2018, , 1.	1.5	1
53	ELECTRON STATES LOCALIZED ON NEUTRAL CLUSTERS CONSISTING OF METAL ATOM AND POLAR MOLECULES. , 1999, , 138-157.		0
54	Modified model of self-consistent field for an electron solvated in a polar liquid. <i>Journal of Experimental and Theoretical Physics</i> , 2003, 97, 566-572.	0.9	0

#	ARTICLE	IF	CITATIONS
55	Estimation of hydrophobic effects using the fundamental measure theory. Biophysics (Russian) Tj ETQq1 1 0.784314.rgBT /Oyerlock 10	0.7	0
56	A universal bridge functional for infinitely diluted solutions. Russian Journal of Physical Chemistry A, 2013, 87, 1598-1599.	0.6	0
57	Hybrid Functions of Lagrange Polynomials and Block-Pulse Functions for Solving Integro-partial Differential Equations. Iranian Journal of Science and Technology, Transaction A: Science, 2018, 42, 2021-2028.	1.5	0
58	CLUSTERIZATION AND CAVITY FORMATION OF INERT GASES ON AN EXCESS ELECTRON. , 1998, , 111-126.		0
59	INTRODUCTION " PHYSICS OF CLUSTERS CLUSTERS IN PLASMA AND GASES. , 1999, , 1-4.		0