# Gennady Chuev

List of Publications by Year
in descending order



| 59 | 1,255 | 471509 17 | 377865 34 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 60 | 60 | 60 | 1132 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. Molecules, 2022, 27, 799. | 3.8 | 5 |
| 2 | CDFTPY: A python package for performing classical density functional theory calculations for molecular liquids. Computer Physics Communications, 2022, 276, 108338. | 7.5 | 6 |
| 3 | Renormalized site density functional theory. Journal of Statistical Mechanics: Theory and Experiment, 2021, 2021, 033205. | 2.3 | 7 |
| 4 | Renormalized site density functional theory for models of ion hydration. Journal of Chemical Physics, 2021, 155, 064501. | 3.0 | 6 |
| 5 | NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102. | 3.0 | 425 |
| 6 | Molecular insight on ion hydration and association in aqueous choline chloride solutions. Journal of Molecular Liquids, 2020, 313, 113563. | 4.9 | 8 |
| 7 | Chemical bond effects in classical site density functional theory of inhomogeneous molecular liquids. Journal of Chemical Physics, 2020, 152, 041101. | 3.0 | 10 |
| 8 | Hydration features of the neurotransmitter acetylcholine. Journal of Molecular Liquids, 2020, 304, 112757. | 4.9 | 17 |
| 9 | Features of local ordering of biocompatible ionic liquids: The case of choline-based amino acid ionic liquids. Journal of Molecular Liquids, 2019, 296, 112081. | 4.9 | 20 |
| 10 | Site density models of inhomogeneous classical molecular liquids. Journal of Statistical Mechanics: Theory and Experiment, 2018, 2018, 093201. | 2.3 | 12 |
| 11 | 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 |
| 12 | 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, , 1. | 1.5 | 1 |
| 13 | Hydration structure of osmolyte TMAO: concentration/pressure-induced response. New Journal of Chemistry, 2017, 41, 1219-1228. | 2.8 | 28 |
| 14 | Local ion hydration structure in aqueous imidazolium-based ionic liquids: The effects of concentration and anion nature. Journal of Molecular Liquids, 2017, 247, 100-108. | 4.9 | 19 |
| 15 | Triangular functions for operational matrix of nonlinear fractional Volterra integral equations. Journal of Applied Mathematics and Computing, 2015, 49, 213-232. | 2.5 | 11 |
| 16 | Exact siteâ€“site bridge functions for dielectric consistent reference interaction site model: A test for ambient water. Journal of Molecular Liquids, 2015, 205, 67-73. | 4.9 | 1 |
| 17 | Extraction of siteâ€“site bridge functions and effective pair potentials from simulations of polar molecular liquids. Journal of Computational Chemistry, 2014, 35, 1010-1023. | 3.3 | 12 |
| 18 | A universal bridge functional for infinitely diluted solutions. Russian Journal of Physical Chemistry A, 2013, 87, 1598-1599. | 0.6 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Electronâ€“electron attraction caused by dispersion forces in metalâ€“ammonia solutions. Chemical Physics Letters, 2013, 556, 138-141. | 2.6 | 1 |
| 20 | Extraction of atomâ€“atom bridge and direct correlation functions from molecular simulations: A test for ambient water. Chemical Physics Letters, 2013, 561-562, 175-178. | 2.6 | 18 |
| 21 | Integral Equation Theory of Molecular Solvation Coupled with Quantum Mechanical/Molecular Mechanics Method in NWChem Package. Journal of Chemical Theory and Computation, 2012, 8, 1246-1254. | 5.3 | 31 |
| 22 | An operational Haar wavelet method for solving fractional Volterra integral equations. International Journal of Applied Mathematics and Computer Science, 2011, 21, 535-547. | 1.5 | 39 |
| 23 | In Silico Screening of Bioactive and Biomimetic Solutes Using Molecular Integral Equation Theory. Current Pharmaceutical Design, 2011, 17, 1695-1708. | 1.9 | 20 |
| 24 | An Accurate Prediction of Hydration Free Energies by Combination of Molecular Integral Equations Theory with Structural Descriptors. Journal of Physical Chemistry B, 2010, 114, 12068-12079. | 2.6 | 74 |
| 25 | Dispersion forces between solvated electrons. Journal of Chemical Physics, 2010, 132, 144504. | 3.0 | 2 |
| 26 | Non-metal-to-metal transition driven by van der Waals forces in an interacting polaronic gas. New Journal of Physics, 2010, 12, 023030. | 2.9 | 2 |
| 27 | Reference interaction site model study of self-aggregating cyanine dyes. Journal of Chemical Physics, 2009, 131, 074503. | 3.0 | 29 |
| 28 | Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. Journal of Computational Chemistry, 2008, 29, 2406-2415. | 3.3 | 38 |
| 29 | Nature of metalâ€“nonmetal transition in metalâ€“ammonia solutions. II. From uniform metallic state to inhomogeneous electronic microstructure. Journal of Chemical Physics, 2008, 128, 144503. | 3.0 | 12 |
| 30 | Comment on â€œModel of saturated lithium ammonia as a single-component liquid metalâ€•[J. Chem. Phys. 124, 074702 (2006)]. Journal of Chemical Physics, 2008, 128, 027101. | 3.0 | 5 |
| 31 | Nature of the metalâ€“nonmetal transition in metalâ€“ammonia solutions. I. Solvated electrons at low metal concentrations. Journal of Chemical Physics, 2007, 127, 244501. | 3.0 | 14 |
| 32 | Improved estimates for hydration free energy obtained by the reference interaction site model. Chemical Physics Letters, 2007, 448, 198-202. | 2.6 | 94 |
| 33 | Herzfeld instability versus Mott transition in metalâ€“ammonia solutions. Comptes Rendus Physique, 2007, 8, 449-455. | 0.9 | 7 |
| 34 | Comparative study of electrostatic solvent response by RISM and PCM methods. International Journal of Quantum Chemistry, 2007, 107, 265-274. | 2.0 | 20 |
| 35 | A structured low-rank wavelet solver for the Ornstein-Zernike integral equation. Computing (Vienna/New York), 2007, 80, 47-73. | 4.8 | 21 |
| 36 | Hydration of Hydrophobic Solutes Treated by the Fundamental Measure Approach. Journal of Physical Chemistry B, 2006, 110, 18496-18503. | 2.6 | 25 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Estimation of hydrophobic effects using the fundamental measure theory. Biophysics (Russian) Tj ETQq1 1 0.784314 rgBT /Overlock 10 | 0.7 | 0 |
| 38 | A probabilistic method for calculating the energy of hydrophobic interactions. Biophysics (Russian) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 | 0.7 | 1 |
| 39 | Wavelet method for solving integral equations of simple liquids. Journal of Molecular Liquids, 2005, 120, 159-162. | 4.9 | 13 |
| 40 | 3D WAVELET TREATMENT OF SOLVATED BIPOLARON AND POLARON. Journal of Theoretical and Computational Chemistry, 2005, 04, 751-767. | 1.8 | 12 |
| 41 | Wavelet treatment of the intrachain correlation functions of homopolymers in dilute solutions. Physical Review E, 2004, 70, 051803. | 2.1 | 8 |
| 42 | Wavelet treatment of structure and thermodynamics of simple liquids. Journal of Chemical Physics, 2004, 120, 1191-1196. | 3.0 | 29 |
| 43 | Density functional method based on wavelets for quantum classical systems. International Journal of Quantum Chemistry, 2004, 100, 539-547. | 2.0 | 14 |
| 44 | Wavelet algorithm for solving integral equations of molecular liquids. A test for the reference interaction site model. Journal of Computational Chemistry, 2004, 25, 1369-1377. | 3.3 | 45 |
| 45 | Density functional theory of bipolarons in polar liquids. Chemical Physics Letters, 2003, 368, 53-58. | 2.6 | 9 |
| 46 | Modified model of self-consistent field for an electron solvated in a polar liquid. Journal of Experimental and Theoretical Physics, 2003, 97, 566-572. | 0.9 | 0 |
| 47 | Density functional study of polarons and bipolarons in polar liquids. Physical Review B, 2003, 67, . | 3.2 | 13 |
| 48 | Wavelet treatment of radial distribution functions of solutes. Physical Review E, 2003, 68, 027702. | 2.1 | 16 |
| 49 | Quantum mechanics of solvated complexes: A test for positronium. International Journal of Quantum Chemistry, 2002, 88, 634-641. | 2.0 | 4 |
| 50 | Mean-field treatment of polarons in strong electrolytes. Physical Review E, 2001, 63, 061204. | 2.1 | 8 |
| 51 | Bipolarons in a KCl melt. Journal of Experimental and Theoretical Physics, 2000, 91, 983-990. | 0.9 | 5 |
| 52 | Superexchange coupling and electron transfer in globular proteins via polaron excitations. Journal of Biological Physics, 2000, 26, 173-184. | 1.5 | 8 |
| 53 | Mean-field theory of an electron solvated in molten salts. Journal of Chemical Physics, 2000, 112, 4707-4715. | 3.0 | 11 |
| 54 | ELECTRON STATES LOCALIZED ON NEUTRAL CLUSTERS CONSISTING OF METAL ATOM AND POLAR MOLECULES. , 1999, , 138-157. | | 0 |

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|---|---|---|---|
| 55 | Statistical theory of a solvated electron in an electrolyte. Journal of Experimental and Theoretical Physics, 1999, 88, 807-814. | 0.9 | 5 |
| 56 | Superexchange coupling and electron transfer in globular proteins via polaron excitations. Journal of Biological Physics, 1999, 24, 245-256. | 1.5 | 1 |
| 57 | INTRODUCTION â€" PHYSICS OF CLUSTERS CLUSTERS IN PLASMA AND GASES. , 1999, , 1-4. | | 0 |
| 58 | CLUSTERIZATION AND CAVITY FORMATION OF INERT GASES ON AN EXCESS ELECTRON. , 1998, , 111-126. | | 0 |
| 59 | A Polaron Model for Electron Transfer in Globular Proteins. Journal of Theoretical Biology, 1993, 163, 51-60. | 1.7 | 13 |