Andriy Kovalenko

List of Publications by Year
in descending order

106 papers	5,851 citations	81434 41 h-index	84171 75 g-index
107 all docs	107 docs citations	107 times ranked	4265 citing authors

#	Article	IF	Citations
1	Response to Comment on â€œDensity Functional Theory and 3D-RISM-KH molecular theory of solvation studies of CO2 reduction on Cu-, Cu2O-, Fe-, and Fe3O4-based nanocatalystsâ€. Journal of Molecular Modeling, 2022, 28, 33.	0.8	2
2	Computational Investigation of the Metal and Ligand Substitution Effects on the Structure and Electronic States of the Phosphoranimide Tetramer Complexes of Cu(I), Ni(I), Co(I), and Fe(I). Inorganic Chemistry, 2022, 61, 1471-1485.	1.9	1
3	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. Journal of Computer-Aided Molecular Design, 2021, 35, 261-269.	1.3	6
4	Cloning and high-level expression of monomeric human superoxide dismutase 1 (SOD1) and its interaction with pyrimidine analogs. PLoS ONE, 2021, 16, e0247684.	1.1	1
5	Biomolecular Simulations with the Three-Dimensional Reference Interaction Site Model with the Kovalenko-Hirata Closure Molecular Solvation Theory. International Journal of Molecular Sciences, 2021, 22, 5061.	1.8	10
6	A 3D-RISM-KH study of liquid nitromethane, nitroethane, and nitrobenzene as solvents. Journal of Molecular Liquids, 2021, 332, 115857.	2.3	3
7	Molecular solvation theory studies of liquid oleyl alcohol and molecular partitioning in water-oleyl alcohol mixture. Chemical Physics Letters, 2021, 777, 138726.	1.2	0
8	Predicting 1,9-Decadieneâ^'Water Partition Coefficients Using the 3D-RISM-KH Molecular Solvation Theory. Physchem, 2021, 1, 215-224.	0.5	0
9	Benchmarking Free Energy Calculations in Liquid Aliphatic Ketone Solvents Using the 3D-RISM-KH Molecular Solvation Theory. J, 2021, 4, 604-613.	0.6	1
10	A molecular solvation theory simulation of liquid alkyl esters of acetic acid with the 3D Reference Interaction Site Model. Journal of Molecular Liquids, 2021, 344, 117763.	2.3	1
11	Density functional theory and 3D-RISM-KH molecular theory of solvation studies of CO2 reduction on Cu-, Cu2O-, Fe-, and Fe3O4-based nanocatalysts. Journal of Molecular Modeling, 2020, 26, 267.	0.8	4
12	Application of the Approximate 3D-Reference Interaction Site Model (RISM) Molecular Solvation Theory to Acetonitrile as Solvent. Journal of Physical Chemistry B, 2020, 124, 4590-4597.	1.2	8
13	Molecular interactions between monoclonal oligomer-specific antibody 5E3 and its amyloid beta cognates. PLoS ONE, 2020, 15, e0232266.	1.1	0
14	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. PLoS ONE, 2019, 14, e0219473.	1.1	22
15	To Pass or Not To Pass: Predicting the Bloodâ€“Brain Barrier Permeability with the 3D-RISM-KH Molecular Solvation Theory. ACS Omega, 2019, 4, 16774-16780.	1.6	28
16	Application of the 3D-RISM-KH molecular solvation theory for DMSO as solvent. Journal of Computer-Aided Molecular Design, 2019, 33, 905-912.	1.3	5
17	The role of hydration effects in 5-fluorouridine binding to SOD1: insight from a new 3D-RISM-KH based protocol for including structural water in docking simulations. Journal of Computer-Aided Molecular Design, 2019, 33, 913-926.	1.3	4
18	Predicting skin permeability using the 3D-RISM-KH theory based solvation energy descriptors for a diverse class of compounds. Journal of Computer-Aided Molecular Design, 2019, 33, 605-611.	1.3	4

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19	Performance of 3D-RISM-KH in Predicting Hydration Free Energy: Effect of Solute Parameters. Journal of Physical Chemistry A, 2019, 123, 4087-4093.	1.1	26
20	Solvent Composition Effects on the Structural Properties of the AÎ²42 Monomer from the 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry B, 2019, 123, 2491-2506.	1.2	6
21	Predicting Bloodâ€“Brain Partitioning of Small Molecules Using a Novel Minimalistic Descriptor-Based Approach via the 3D-RISM-KH Molecular Solvation Theory. ACS Omega, 2019, 4, 3055-3060.	1.6	12
22	Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors. Journal of Computer-Aided Molecular Design, 2019, 33, 965-971.	1.3	7
23	Enhanced solvation force extrapolation for speeding up molecular dynamics simulations of complex biochemical liquids. Journal of Chemical Physics, 2019, 151, 214102.	1.2	5
24	Tryptophan 32 mediates SOD1 toxicity in a in vivo motor neuron model of ALS and is a promising target for small molecule therapeutics. Neurobiology of Disease, 2019, 124, 297-310.	2.1	25
25	Computational and Experimental Investigations of the Role of Water and Alcohols in the Desorption of Heterocyclic Aromatic Compounds from Kaolinite in Toluene. Journal of Physical Chemistry C, 2018, 122, 10377-10391.	1.5	4
26	Multiscale methods framework: self-consistent coupling of molecular theory of solvation with quantum chemistry, molecular simulations, and dissipative particle dynamics. Physical Chemistry Chemical Physics, 2018, 20, 2947-2969.	1.3	24
27	Multiscale Modeling of Solvation. , 2017, , 95-139.		17
28	Predicting Accurate Solvation Free Energy in n-Octanol Using 3D-RISM-KH Molecular Theory of Solvation: Making Right Choices. Journal of Physical Chemistry B, 2017, 121, 9268-9273.	1.2	22
29	Effective Interactions and Adsorption of Heterocyclic Aromatic Hydrocarbons in Kaolinite Organic Solutions Studied by 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry C, 2017, 121, 22092-22104.	1.5	6
30	Initial Structural Models of the AÎ²42 Dimer from Replica Exchange Molecular Dynamics Simulations. ACS Omega, 2017, 2, 7621-7636.	1.6	10
31	A closure relation to molecular theory of solvation for macromolecules. Journal of Physics Condensed Matter, 2016, 28, 404003.	0.7	20
32	SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. Journal of Computer-Aided Molecular Design, 2016, 30, 1115-1127.	1.3	29
33	A 3D-RISM-KH Molecular Theory of Solvation Study of the Effective Stacking Interactions of Kaolinite Nanoparticles in Aqueous Electrolyte Solution Containing Additives. Journal of Physical Chemistry C, 2016, 120, 21344-21357.	1.5	8
34	Cellulose Aggregation under Hydrothermal Pretreatment Conditions. Biomacromolecules, 2016, 17, 2582-2590.	2.6	62
35	Adsorption of Bitumen Model Compounds on Kaolinite in Liquid and Supercritical Carbon Dioxide Solvents: A Study by Periodic Density Functional Theory and Molecular Theory of Solvation. Energy & Fuels, 2015, 29, 2853-2863.	2.5	12
36	Supramolecular Interactions in Secondary Plant Cell Walls: Effect of Lignin Chemical Composition Revealed with the Molecular Theory of Solvation. Journal of Physical Chemistry Letters, 2015, 6, 206-211.	2.1	60

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37	Role of Water in Ligand Binding to Maltose-Binding Protein: Insight from a New Docking Protocol Based on the 3D-RISM-KH Molecular Theory of Solvation. Journal of Chemical Information and Modeling, 2015, 55, 317-328.	2.5	20
38	Octanolâ€“Water Partition Coefficient from 3D-RISM-KH Molecular Theory of Solvation with Partial Molar Volume Correction. Journal of Physical Chemistry B, 2015, 119, 5588-5597.	1.2	39
39	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.	2.3	36
40	Dissipative Particle Dynamics with an Effective Pair Potential from Integral Equation Theory of Molecular Liquids. Journal of Physical Chemistry B, 2014, 118, 12034-12049.	1.2	9
41	Moleculeâ€“Surface Recognition between Heterocyclic Aromatic Compounds and Kaolinite in Toluene Investigated by Molecular Theory of Solvation and Thermodynamic and Kinetic Experiments. Journal of Physical Chemistry C, 2014, 118, 23821-23834.	1.5	23
42	Adsorption of Indole on Kaolinite in Nonaqueous Media: Organoclay Preparation and Characterization, and 3D-RISM-KH Molecular Theory of Solvation Investigation. Journal of Physical Chemistry C, 2013, 117, 18556-18566.	1.5	34
43	Multiscale modeling of solvation in chemical and biological nanosystems and in nanoporous materials. Pure and Applied Chemistry, 2013, 85, 159-199.	0.9	58
44	Generalised canonicalâ€“isokinetic ensemble: speeding up multiscale molecular dynamics and coupling with 3D molecular theory of solvation. Molecular Simulation, 2013, 39, 25-48.	0.9	17
45	Plant Biomass Recalcitrance: Effect of Hemicellulose Composition on Nanoscale Forces that Control Cell Wall Strength. Journal of the American Chemical Society, 2013, 135, 19048-19051.	6.6	108
46	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.	1.2	20
47	3D-RISM-D‹scp›ock‹/scp›: A New Fragment-Based Drug Design Protocol. Journal of Chemical Theory and Computation, 2012, 8, 3356-3372.	2.3	37
48	Molecular theory of solvation for supramolecules and soft matter structures: application to ligand binding, ion channels, and oligomeric polyelectrolyte gelators. Soft Matter, 2012, 8, 1508-1520.	1.2	44
49	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.	2.3	12
50	Interpretation of atomic motion in flexible molecules: Accelerating molecular dynamics simulations. Physical Review E, 2012, 85, 026706.	0.8	7
51	Efficient treatment of solvation shells in 3D molecular theory of solvation. Journal of Computational Chemistry, 2012, 33, 1478-1494.	1.5	49
52	3D-RISM-KH approach for biomolecular modelling at nanoscale: thermodynamics of fibril formation and beyond. Molecular Simulation, 2011, 37, 718-728.	0.9	16
53	Calculation of Local Water Densities in Biological Systems: A Comparison of Molecular Dynamics Simulations and the 3D-RISM-KH Molecular Theory of Solvation. Journal of Physical Chemistry B, 2011, 115, 319-328.	1.2	80
54	Diazonium-Derived Aryl Films on Gold Nanoparticles: Evidence for a Carbonâ€“Gold Covalent Bond. ACS Nano, 2011, 5, 4219-4227.	7.3	189

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55	Multiscale methods for nanochemistry and biophysics in solution. Journal of Molecular Liquids, 2011, 164, 101-112.	2.3	18
56	Spatial Decomposition of Solvation Free Energy Based on the 3D Integral Equation Theory of Molecular Liquid: Application to Miniproteins. Journal of Physical Chemistry B, 2011, 115, 310-318.	1.2	24
57	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. II. Canonical and isokinetic ensembles. Journal of Chemical Physics, 2011, 135, 234107.	1.2	12
58	Self-Assembly of a Water-Soluble Tricyclic Heterocycle into J-Type Rosette Nanotubes. Materials Research Society Symposia Proceedings, 2011, 1312, 1.	0.1	0
59	Multiple time scale molecular dynamics for fluids with orientational degrees of freedom. I. Microcanonical ensemble. Journal of Chemical Physics, 2011, 135, 114110.	1.2	9
60	Structural Water Drives Selfâ€assembly of Organic Rosette Nanotubes and Holds Host Atoms in the Channel. ChemPhysChem, 2010, 11, 361-367.	1.0	43
61	Selfâ€Consistent Field Modeling of Threeâ€Dimensional Morphologies of Branched Lipid Surfactant at Airâ€Water Interface. Macromolecular Theory and Simulations, 2010, 19, 228-239.	0.6	3
62	Modeling Solvatochromic Shifts Using the Orbital-Free Embedding Potential at Statistically Mechanically Averaged Solvent Density. Journal of Physical Chemistry A, 2010, 114, 6082-6096.	1.1	84
63	Association Thermodynamics and Conformational Stability of Î²-Sheet Amyloid Î²(17-42) Oligomers: Effects of E22Q (Dutch) Mutation and Charge Neutralization. Biophysical Journal, 2010, 98, 282-296.	0.2	49
64	One-Pot Nucleation, Growth, Morphogenesis, and Passivation of 1.4 nm Au Nanoparticles on Self-Assembled Rosette Nanotubes. Journal of the American Chemical Society, 2010, 132, 32-33.	6.6	47
65	Computational and Experimental Study of the Structure, Binding Preferences, and Spectroscopy of Nickel(II) and Vanadyl Porphyrins in Petroleum. Journal of Physical Chemistry B, 2010, 114, 2180-2188.	1.2	55
66	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2010, 6, 607-624.	2.3	232
67	Electronic Characteristics and Charge Transport Mechanisms for Large Area Aromatic Molecular Junctions. Journal of Physical Chemistry C, 2010, 114, 15806-15815.	1.5	83
68	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	1.2	129
69	Supramolecular Synthesis of Solidâ€State Tapes Through Molecular Facial Selfâ€Recognition. Helvetica Chimica Acta, 2009, 92, 1963-1972.	1.0	1
70	On variational estimates for exchange-correlation interaction obtained within super-CI approach to MCSCF approximation. International Journal of Quantum Chemistry, 2009, 109, 1672-1675.	1.0	4
71	Thermodynamic dependences of slip length for nanofluidic flows over crystalline surfaces: Predictions of molecular theory of solvation. International Journal of Quantum Chemistry, 2009, 109, 1666-1671.	1.0	6
72	Ab Initio Study of Ionic Liquids by KS-DFT/3D-RISM-KH Theory. Journal of Physical Chemistry B, 2009, 113, 3536-3542.	1.2	43

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73	Spatial Decomposition Analysis of the Thermodynamics of Cyclodextrin Complexation. Journal of Chemical Theory and Computation, 2009, 5, 1723-1730.	2.3	24
74	Ligand Mapping on Protein Surfaces by the 3D-RISM Theory: Toward Computational Fragment-Based Drug Design. Journal of the American Chemical Society, 2009, 131, 12430-12440.	6.6	109
75	Molecular Recognition in Biomolecules Studied by Statistical-Mechanical Integral-Equation Theory of Liquids. Journal of Physical Chemistry B, 2009, 113, 873-886.	1.2	114
76	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. Journal of Physical Chemistry C, 2008, 112, 6794-6810.	1.5	55
77	Hydration Effects on the HET-s Prion and Amyloid-Î² Fibrillous Aggregates, Studied with Three-Dimensional Molecular Theory of Solvation. Biophysical Journal, 2008, 95, 4540-4548.	0.2	45
78	Multiscale modelling of asphaltene disaggregation. Molecular Simulation, 2008, 34, 953-960.	0.9	24
79	Hierarchical Self-Assembly of Organic Prolate Nanospheroids from Hydrophobic Rosette Nanotubes. Langmuir, 2008, 24, 4447-4450.	1.6	34
80	Molecular theory of hydrodynamic boundary conditions in nanofluidics. Journal of Chemical Physics, 2008, 129, 134701.	1.2	37
81	Theoretical analysis on changes in thermodynamic quantities upon protein folding: Essential role of hydration. Journal of Chemical Physics, 2007, 126, 225102.	1.2	75
82	Molecular Basis for Water-Promoted Supramolecular Chirality Inversion in Helical Rosette Nanotubes. Journal of the American Chemical Society, 2007, 129, 5735-5743.	6.6	184
83	Three-Dimensional Distribution Function Theory for the Prediction of Proteinâ^'Ligand Binding Sites and Affinities:â€‰ Application to the Binding of Noble Gases to Hen Egg-White Lysozyme in Aqueous Solution. Journal of Physical Chemistry B, 2007, 111, 11585-11591.	1.2	41
84	Evaluation of the SCF Combination of KS-DFT and 3D-RISM-KH; Solvation Effect on Conformational Equilibria, Tautomerization Energies, and Activation Barriers. Journal of Chemical Theory and Computation, 2007, 3, 458-476.	2.3	57
85	Microtubule Stability Studied by Three-Dimensional Molecular Theory of Solvation. Biophysical Journal, 2007, 92, 394-403.	0.2	57
86	Theoretical study of the partial molar volume change associated with the pressureâ€‰induced structural transition of ubiquitin. Protein Science, 2007, 16, 1927-1933.	3.1	53
87	A theoretical analysis on hydration thermodynamics of proteins. Journal of Chemical Physics, 2006, 125, 024911.	1.2	139
88	Self-Consistent Combination of the Three-Dimensional RISM Theory of Molecular Solvation with Analytical Gradients and the Amsterdam Density Functional Package. Journal of Physical Chemistry A, 2006, 110, 6083-6090.	1.1	92
89	Theoretical Study of Volume Changes Accompanying Xenonâ^'Lysozyme Binding:Â Implications for the Molecular Mechanism of Pressure Reversal of Anesthesia. Journal of Physical Chemistry B, 2006, 110, 12149-12154.	1.2	18
90	1P093 A Theoretical Analysis on the Free Energy Changes Associated with Protein Folding(3. Protein) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Butsuri, 2006, 46, S170.	0.0	0

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91	Locating missing water molecules in protein cavities by the three-dimensional reference interaction site model theory of molecular solvation. Proteins: Structure, Function and Bioinformatics, 2006, 66, 804-813.	1.5	89
92	A molecular theory of liquid interfaces. Physical Chemistry Chemical Physics, 2005, 7, 1785.	1.3	41
93	Helical Rosette Nanotubes with Tunable Stability and Hierarchy. Journal of the American Chemical Society, 2005, 127, 8307-8309.	6.6	134
94	Water Molecules in a Protein Cavity Detected by a Statisticalâ˜Mechanical Theory. Journal of the American Chemical Society, 2005, 127, 15334-15335.	6.6	147
95	Three-dimensional Rism Theory for Molecular Liquids and Solid-Liquid Interfaces. , 2004, , 169-275.		39
96	Compressibility oftert-Butyl Alcohol-Water Mixtures: The Rism Theory. Journal of Theoretical and Computational Chemistry, 2003, 02, 193-203.	1.8	37
97	TOWARDS A MOLECULAR THEORY FOR THE VAN DER WAALSâ€“MAXWELL DESCRIPTION OF FLUID PHASE TRANSITIONS. Journal of Theoretical and Computational Chemistry, 2002, 01, 381-406.	1.8	41
98	Structure of tert-Butyl Alcoholâ˜Water Mixtures Studied by the RISM Theory. Journal of Physical Chemistry B, 2002, 106, 5042-5049.	1.2	126
99	Theoretical study for volume changes associated with the helix-coil transition of peptides. Biopolymers, 2001, 59, 512-519.	1.2	53
100	Theoretical study for partial molar volume of amino acids and polypeptides by the three-dimensional reference interaction site model. Journal of Chemical Physics, 2001, 114, 9506-9511.	1.2	84
101	Potentials of mean force of simple ions in ambient aqueous solution. II. Solvation structure from the three-dimensional reference interaction site model approach, and comparison with simulations. Journal of Chemical Physics, 2000, 112, 10403-10417.	1.2	127
102	Potentials of mean force of simple ions in ambient aqueous solution. I. Three-dimensional reference interaction site model approach. Journal of Chemical Physics, 2000, 112, 10391-10402.	1.2	258
103	Solution of three-dimensional reference interaction site model and hypernetted chain equations for simple point charge water by modified method of direct inversion in iterative subspace. Journal of Computational Chemistry, 1999, 20, 928-936.	1.5	224
104	Self-consistent description of a metalâ€“water interface by the Kohnâ€“Sham density functional theory and the three-dimensional reference interaction site model. Journal of Chemical Physics, 1999, 110, 10095-10112.	1.2	608
105	Potential of Mean Force between Two Molecular Ions in a Polar Molecular Solvent: A Study by the Three-Dimensional Reference Interaction Site Model. Journal of Physical Chemistry B, 1999, 103, 7942-7957.	1.2	181
106	Three-dimensional density profiles of water in contact with a solute of arbitrary shape: a RISM approach. Chemical Physics Letters, 1998, 290, 237-244.	1.2	409