Sergey Gusarov

List of Publications by Citations

55 papers	1,666 citations	24 h-index	40 g-index
64 ext. papers	1,894 ext. citations	4.2 avg, IF	4.69 L-index

#	Paper	IF	Citations
55	Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber. *Journal of Chemical Theory and Computation*, **2010**, 6, 607-624	6.4	197
54	An MM/3D-RISM approach for ligand binding affinities. *Journal of Physical Chemistry B*, **2010**, 114, 8505-16	3.4	117
53	Plant biomass recalcitrance: effect of hemicellulose composition on nanoscale forces that control cell wall strength. *Journal of the American Chemical Society*, **2013**, 135, 19048-51	16.4	82
52	Density Functional Theory Investigation of the Contributions of π-Stacking and Hydrogen-Bonding Interactions to the Aggregation of Model Asphaltene Compounds. *Energy & Fuels*, **2012**, 26, 2727-2735	4.1	81
51	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, 6083-90	2.8	75
50	Modeling solvatochromic shifts using the orbital-free embedding potential at statistically mechanically averaged solvent density. *Journal of Physical Chemistry A*, **2010**, 114, 6082-96	2.8	74
49	Electronic Characteristics and Charge Transport Mechanisms for Large Area Aromatic Molecular Junctions. *Journal of Physical Chemistry C*, **2010**, 114, 15806-15815	3.8	73
48	Single-side-hydrogenated graphene: Density functional theory predictions. *Physical Review B*, **2011**, 84,	3.3	71
47	Optical control of selectivity of high rate CO2 photoreduction via interband- or hot electron Z-scheme reaction pathways in Au-TiO2 plasmonic photonic crystal photocatalyst. *Applied Catalysis B: Environmental*, **2020**, 267, 118644	21.8	56
46	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, 458-76	6.4	55
45	Microtubule stability studied by three-dimensional molecular theory of solvation. *Biophysical Journal*, **2007**, 92, 394-403	2.9	53
44	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. *Theoretical Chemistry Accounts*, **2004**, 112, 84-94	1.9	52
43	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, 2180-8	3.4	47
42	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. *Molecular Physics*, **2004**, 102, 2207-2216	1.7	46
41	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, 206-11	6.4	45
40	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. *Journal of Physical Chemistry C*, **2008**, 112, 6794-6810	3.8	45
39	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	3.6	43

38	Efficient treatment of solvation shells in 3D molecular theory of solvation. *Journal of Computational Chemistry*, **2012**, 33, 1478-94	3.5	42
37	Ab initio study of ionic liquids by KS-DFT/3D-RISM-KH theory. *Journal of Physical Chemistry B*, **2009**, 113, 3536-42	3.4	40
36	Computational study of the effect of dispersion interactions on the thermochemistry of aggregation of fused polycyclic aromatic hydrocarbons as model asphaltene compounds in solution. *Journal of Physical Chemistry A*, **2014**, 118, 896-908	2.8	37
35	Consistently High Values in p-i-n Type Perovskite Solar Cells Using Ni-Doped NiO Nanomesh as the Hole Transporting Layer. *ACS Applied Materials & Interfaces*, **2020**, 12, 11467-11478	9.5	33
34	Donor-acceptor small molecules for organic photovoltaics: single-atom substitution (Se or S). *ACS Applied Materials & Interfaces*, **2015**, 7, 8188-99	9.5	31
33	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	3.8	30
32	Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. *Journal of Physical Chemistry B*, **2009**, 113, 9958-67	3.4	25
31	MoleculeSurface 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	3.8	21
30	Multiscale modelling of asphaltene disaggregation. *Molecular Simulation*, **2008**, 34, 953-960	2	21
29	Density functional theory investigation of the effect of axial coordination and annelation on the absorption spectroscopy of nickel(II) and vanadyl porphyrins relevant to bitumen and crude oils. *Canadian Journal of Chemistry*, **2013**, 91, 872-878	0.9	19
28	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	3.6	17
27	A closure relation to molecular theory of solvation for macromolecules. *Journal of Physics Condensed Matter*, **2016**, 28, 404003	1.8	15
26	Modelling of bitumen fragment adsorption on Cu+ and Ag+ exchanged zeolite nanoparticles. *Molecular Simulation*, **2008**, 34, 943-951	2	13
25	Development of Fukui Function Based Descriptors for a Machine Learning Study of CO2 Reduction. *Journal of Physical Chemistry C*, **2020**, 124, 10079-10084	3.8	12
24	Photocatalytic Mechanism Control and Study of Carrier Dynamics in CdS@CN Core-Shell Nanowires. *ACS Applied Materials & Interfaces*, **2021**, 13, 47418-47439	9.5	11
23	Electric Interfacial Layer of Modified Cellulose Nanocrystals in Aqueous Electrolyte Solution: Predictions by the Molecular Theory of Solvation. *Langmuir*, **2015**, 31, 7106-16	4	10
22	Theoretical Modeling of Tunneling Barriers in Carbon-Based Molecular Electronic Junctions. *Journal of Physical Chemistry C*, **2015**, 119, 11286-11295	3.8	9
21	Harvesting Hot Holes in Plasmon-Coupled Ultrathin Photoanodes for High-Performance Photoelectrochemical Water Splitting. *ACS Applied Materials & Interfaces*, **2021**, 13, 42741-42752	9.5	9

20	Multi-scale modeling and synthesis of polyester ionomers. *Physical Chemistry Chemical Physics*, **2013**, 15, 6128-38	3.6	8
19	Dissipative particle dynamics with an effective pair potential from integral equation theory of molecular liquids. *Journal of Physical Chemistry B*, **2014**, 118, 12034-49	3.4	7
18	Multiscale modeling of active layer of hybrid organic-inorganic solar cells for photovoltaic applications by means of density functional theory and integral equation theory of molecular liquids. *Journal of Molecular Liquids*, **2019**, 289, 110997	6	6
17	CVD grown nitrogen doped graphene is an exceptional visible-light driven photocatalyst for surface catalytic reactions. *2D Materials*, **2020**, 7, 015002	5.9	6
16	COSMO-RS-Based Descriptors for the Machine Learning-Enabled Screening of Nucleotide Analogue Drugs against SARS-CoV-2. *Journal of Physical Chemistry Letters*, **2020**, 11, 9408-9414	6.4	6
15	Synthesis and Characterization of Zinc Phthalocyanine-Cellulose Nanocrystal (CNC) Conjugates: Toward Highly Functional CNCs. *ACS Applied Materials & Interfaces*, **2020**, 12, 43992-44006	9.5	4
14	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	3.8	3
13	On variational estimates for exchange-correlation interaction obtained within super-CI approach to MCSCF approximation. *International Journal of Quantum Chemistry*, **2009**, 109, 1672-1675	2.1	3
12	Development of additive isotropic site potential for exchange-repulsion energy, based on intermolecular perturbation theory. *Canadian Journal of Chemistry*, **2009**, 87, 1727-1732	0.9	3
11	The Effect of Molecular Structure and Environment on the Miscibility and Diffusivity in Polythiophene-Methanofullerene Bulk Heterojunctions: Theory and Modeling with the RISM Approach. *Polymers*, **2016**, 8,	4.5	3
10	Koopmans multiconfigurational self-consistent field (MCSCF) Fukui functions and MCSCF perturbation theory. *Canadian Journal of Chemistry*, **2013**, 91, 886-893	0.9	2
9	Comment on "Density functional theory and 3D-RISM-KH molecular theory of solvation studies of CO reduction on Cu-, CuO-, Fe-, and FeO-based nanocatalysts". *Journal of Molecular Modeling*, **2021**, 27, 344	2	2
8	Organic-Inorganic Nanohybrid Materials for Photovoltaic Applications. *ECS Transactions*, **2018**, 85, 543-550	1	1
7	TiO2-HfN Radial Nano-Heterojunction: A Hot Carrier Photoanode for Sunlight-Driven Water-Splitting. *Catalysts*, **2021**, 11, 1374	4	1
6	Extended Koopmans Approximation for CASDFT Exchange-Correlation Functional. *Journal of Applied Mathematics and Physics*, **2018**, 06, 1242-1246	0.3	0
5	Modeling the interaction of SARS-CoV-2 binding to the ACE2 receptor via molecular theory of solvation. *New Journal of Chemistry*, **2021**, 45, 15448-15457	3.6	0
4	Hot hole transfer from Ag nanoparticles to multiferroic YMn2O5 nanowires enables superior photocatalytic activity. *Journal of Materials Chemistry C*, **2022**, 10, 4128-4139	7.1	0
3	Experimental and Computational Synergistic Design of Cu and Fe Catalysts for the Reverse Water Gas Shift: A Review. *ACS Catalysis*,6887-6905	13.1	0

List of Publications

2 Density Functional Investigation of Charge Transfer in Organic Solar Cells. *ECS Transactions*, **2011**, 41, 129-134 1

1 A reply to: "Response to Comment on "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*, **2022**, 28, 114 2