

Sergey Gusarov

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Hot hole transfer from Ag nanoparticles to multiferroic YMn ₂ O ₅ nanowires enables superior photocatalytic activity. <i>Journal of Materials Chemistry C</i> , 2022 , 10, 4128-4139	7.1	0
54	A reply to: "Response to Comment on "Density Functional Theory and 3D-RISM-KH molecular theory of solvation studies of CO ₂ reduction on Cu-, Cu ₂ O-, Fe-, and Fe ₃ O ₄ -based nanocatalysts"".. <i>Journal of Molecular Modeling</i> , 2022 , 28, 114	2	
53	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". <i>Journal of Molecular Modeling</i> , 2021 , 27, 344	2	2
52	TiO ₂ -HfN Radial Nano-Heterojunction: A Hot Carrier Photoanode for Sunlight-Driven Water-Splitting. <i>Catalysts</i> , 2021 , 11, 1374	4	1
51	Photocatalytic Mechanism Control and Study of Carrier Dynamics in CdS@CN Core-Shell Nanowires. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 47418-47439	9.5	11
50	Harvesting Hot Holes in Plasmon-Coupled Ultrathin Photoanodes for High-Performance Photoelectrochemical Water Splitting. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 42741-42752	9.5	9
49	Modeling the interaction of SARS-CoV-2 binding to the ACE2 receptor via molecular theory of solvation. <i>New Journal of Chemistry</i> , 2021 , 45, 15448-15457	3.6	0
48	Synthesis and Characterization of Zinc Phthalocyanine-Cellulose Nanocrystal (CNC) Conjugates: Toward Highly Functional CNCs. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 43992-44006	9.5	4
47	Optical control of selectivity of high rate CO ₂ photoreduction via interband- or hot electron Z-scheme reaction pathways in Au-TiO ₂ plasmonic photonic crystal photocatalyst. <i>Applied Catalysis B: Environmental</i> , 2020 , 267, 118644	21.8	56
46	CVD grown nitrogen doped graphene is an exceptional visible-light driven photocatalyst for surface catalytic reactions. <i>2D Materials</i> , 2020 , 7, 015002	5.9	6
45	Consistently High Values in p-i-n Type Perovskite Solar Cells Using Ni-Doped NiO Nanomesh as the Hole Transporting Layer. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 11467-11478	9.5	33
44	COSMO-RS-Based Descriptors for the Machine Learning-Enabled Screening of Nucleotide Analogue Drugs against SARS-CoV-2. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9408-9414	6.4	6
43	Development of Fukui Function Based Descriptors for a Machine Learning Study of CO ₂ Reduction. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 10079-10084	3.8	12
42	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. <i>Journal of Molecular Liquids</i> , 2019 , 289, 110997	6	6
41	Computational and Experimental Investigations of the Role of Water and Alcohols in the Desorption of Heterocyclic Aromatic Compounds from Kaolinite in Toluene. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 10377-10391	3.8	3
40	Multiscale methods framework: self-consistent coupling of molecular theory of solvation with quantum chemistry, molecular simulations, and dissipative particle dynamics. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 2947-2969	3.6	17
39	Organic-Inorganic Nanohybrid Materials for Photovoltaic Applications. <i>ECS Transactions</i> , 2018 , 85, 543-550		1

38	Extended Koopmans's Approximation for CASDFT Exchange-Correlation Functional. <i>Journal of Applied Mathematics and Physics</i> , 2018 , 06, 1242-1246	0.3	0
37	The Effect of Molecular Structure and Environment on the Miscibility and Diffusivity in Polythiophene-Methanofullerene Bulk Heterojunctions: Theory and Modeling with the RISM Approach. <i>Polymers</i> , 2016 , 8,	4.5	3
36	A closure relation to molecular theory of solvation for macromolecules. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 404003	1.8	15
35	Electric Interfacial Layer of Modified Cellulose Nanocrystals in Aqueous Electrolyte Solution: Predictions by the Molecular Theory of Solvation. <i>Langmuir</i> , 2015 , 31, 7106-16	4	10
34	Donor-acceptor small molecules for organic photovoltaics: single-atom substitution (Se or S). <i>ACS Applied Materials & Interfaces</i> , 2015 , 7, 8188-99	9.5	31
33	Theoretical Modeling of Tunneling Barriers in Carbon-Based Molecular Electronic Junctions. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 11286-11295	3.8	9
32	Supramolecular Interactions in Secondary Plant Cell Walls: Effect of Lignin Chemical Composition Revealed with the Molecular Theory of Solvation. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 206-11	6.4	45
31	Computational study of the effect of dispersion interactions on the thermochemistry of aggregation of fused polycyclic aromatic hydrocarbons as model asphaltene compounds in solution. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 896-908	2.8	37
30	Dissipative particle dynamics with an effective pair potential from integral equation theory of molecular liquids. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 12034-49	3.4	7
29	Molecule-Surface Recognition between Heterocyclic Aromatic Compounds and Kaolinite in Toluene Investigated by Molecular Theory of Solvation and Thermodynamic and Kinetic Experiments. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23821-23834	3.8	21
28	Adsorption of Indole on Kaolinite in Nonaqueous Media: Organoclay Preparation and Characterization, and 3D-RISM-KH Molecular Theory of Solvation Investigation. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 18556-18566	3.8	30
27	Koopmans's multiconfigurational self-consistent field (MCSCF) Fukui functions and MCSCF perturbation theory. <i>Canadian Journal of Chemistry</i> , 2013 , 91, 886-893	0.9	2
26	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. <i>Canadian Journal of Chemistry</i> , 2013 , 91, 872-878	0.9	19
25	Multi-scale modeling and synthesis of polyester ionomers. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 6128-38	3.6	8
24	Plant biomass recalcitrance: effect of hemicellulose composition on nanoscale forces that control cell wall strength. <i>Journal of the American Chemical Society</i> , 2013 , 135, 19048-51	16.4	82
23	Density Functional Theory Investigation of the Contributions of π -Stacking and Hydrogen-Bonding Interactions to the Aggregation of Model Asphaltene Compounds. <i>Energy & Fuels</i> , 2012 , 26, 2727-2735	4.1	81
22	Molecular theory of solvation for supramolecules and soft matter structures: application to ligand binding, ion channels, and oligomeric polyelectrolyte gelators. <i>Soft Matter</i> , 2012 , 8, 1508-1520	3.6	43
21	Efficient treatment of solvation shells in 3D molecular theory of solvation. <i>Journal of Computational Chemistry</i> , 2012 , 33, 1478-94	3.5	42

20	Single-side-hydrogenated graphene: Density functional theory predictions. <i>Physical Review B</i> , 2011 , 84,	3.3	71
19	Density Functional Investigation of Charge Transfer in Organic Solar Cells. <i>ECS Transactions</i> , 2011 , 41, 129-134	1	
18	Modeling solvatochromic shifts using the orbital-free embedding potential at statistically mechanically averaged solvent density. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 6082-96	2.8	74
17	Computational and experimental study of the structure, binding preferences, and spectroscopy of nickel(II) and vanadyl porphyrins in petroleum. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 2180-8	3.4	47
16	Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 607-624	6.4	197
15	Electronic Characteristics and Charge Transport Mechanisms for Large Area Aromatic Molecular Junctions. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 15806-15815	3.8	73
14	An MM/3D-RISM approach for ligand binding affinities. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 8505-164	3.4	117
13	On variational estimates for exchange-correlation interaction obtained within super-CI approach to MCSCF approximation. <i>International Journal of Quantum Chemistry</i> , 2009 , 109, 1672-1675	2.1	3
12	Ab initio study of ionic liquids by KS-DFT/3D-RISM-KH theory. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 3536-42	3.4	40
11	Development of additive isotropic site potential for exchange-repulsion energy, based on intermolecular perturbation theory. <i>Canadian Journal of Chemistry</i> , 2009 , 87, 1727-1732	0.9	3
10	Electronic structure, binding energy, and solvation structure of the streptavidin-biotin supramolecular complex: ONIOM and 3D-RISM study. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 9958-6734	3.4	25
9	Theoretical Modeling of Zeolite Nanoparticle Surface Acidity for Heavy Oil Upgrading. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 6794-6810	3.8	45
8	Multiscale modelling of asphaltene disaggregation. <i>Molecular Simulation</i> , 2008 , 34, 953-960	2	21
7	Modelling of bitumen fragment adsorption on Cu ⁺ and Ag ⁺ exchanged zeolite nanoparticles. <i>Molecular Simulation</i> , 2008 , 34, 943-951	2	13
6	Evaluation of the SCF Combination of KS-DFT and 3D-RISM-KH; Solvation Effect on Conformational Equilibria, Tautomerization Energies, and Activation Barriers. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 458-76	6.4	55
5	Microtubule stability studied by three-dimensional molecular theory of solvation. <i>Biophysical Journal</i> , 2007 , 92, 394-403	2.9	53
4	Self-consistent combination of the three-dimensional RISM theory of molecular solvation with analytical gradients and the Amsterdam density functional package. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 6083-90	2.8	75
3	Correlation potentials for a multiconfigurational-based density functional theory with exact exchange. <i>Theoretical Chemistry Accounts</i> , 2004 , 112, 84-94	1.9	52

2	Using on-top pair density for construction of correlation functionals for multideterminant wave functions. <i>Molecular Physics</i> , 2004 , 102, 2207-2216	1.7	46
1	Experimental and Computational Synergistic Design of Cu and Fe Catalysts for the Reverse Water-Gas Shift: A Review. <i>ACS Catalysis</i> , 6887-6905	13.1	0