

Daria B Kokh

List of Publications by Citations

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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.

58
papers

1,769
citations

25
h-index

41
g-index

64
ext. papers

2,235
ext. citations

5.3
avg, IF

4.86
L-index

#	Paper	IF	Citations
58	Protein Binding Pocket Dynamics. <i>Accounts of Chemical Research</i> , 2016 , 49, 809-15	24.3	156
57	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. <i>Drug Discovery Today</i> , 2017 , 22, 896-911	8.8	113
56	Docking of ubiquitin to gold nanoparticles. <i>ACS Nano</i> , 2012 , 6, 9863-78	16.7	112
55	Modeling and simulation of protein-surface interactions: achievements and challenges. <i>Quarterly Reviews of Biophysics</i> , 2016 , 49, e4	7	112
54	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. <i>Nature Communications</i> , 2017 , 8, 2276	17.4	101
53	Estimation of Drug-Target Residence Times by ϵ Random Acceleration Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3859-3869	6.4	95
52	New approaches for computing ligand-receptor binding kinetics. <i>Current Opinion in Structural Biology</i> , 2018 , 49, 1-10	8.1	80
51	High throughput in-silico screening against flexible protein receptors. <i>Journal of Cheminformatics</i> , 2010 , 2,	8.6	78
50	On the ultraviolet photofragmentation of hydrogen iodide. <i>Journal of Chemical Physics</i> , 2000 , 113, 6174-6185	5.9	59
49	TRAPP: a tool for analysis of transient binding pockets in proteins. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1235-52	6.1	52
48	ProMetCS: An Atomistic Force Field for Modeling Protein-Metal Surface Interactions in a Continuum Aqueous Solvent. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1753-68	6.4	51
47	SDA 7: A modular and parallel implementation of the simulation of diffusional association software. <i>Journal of Computational Chemistry</i> , 2015 , 36, 1631-45	3.5	46
46	A comparative study of the electron distribution function in the positive columns in and /He dc glow discharges by optical spectroscopy and probes. <i>Plasma Sources Science and Technology</i> , 1998 , 7, 298-309	3.5	46
45	Flexible side chain models improve enrichment rates in in silico screening. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 5919-31	8.3	42
44	Receptor flexibility in small-molecule docking calculations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011 , 1, 298-314	7.9	38
43	Absolute calibration of the efficiency of a VUV-monochromator/detector system in the range 110 - 450 nm. <i>Measurement Science and Technology</i> , 1997 , 8, 773-781	2	36
42	A quantitative, real-time assessment of binding of peptides and proteins to gold surfaces. <i>Chemistry - A European Journal</i> , 2011 , 17, 1327-36	4.8	34

41	Protein-surface interactions: challenging experiments and computations. <i>Journal of Molecular Recognition</i> , 2010 , 23, 259-62	2.6	33
40	Ab initio study of spectroscopic and radiative characteristics of ion-pair states of the Cl ₂ molecule. <i>Journal of Chemical Physics</i> , 2001 , 115, 9298-9310	3.9	31
39	Diffusion and association processes in biological systems: theory, computation and experiment. <i>BMC Biophysics</i> , 2011 , 4, 2	0	29
38	Relativistic configuration interaction study of the ClF molecule and its emission spectra from 0+ ion-pair states. <i>Journal of Chemical Physics</i> , 2000 , 112, 2274-2284	3.9	29
37	Theoretical study of the UV photodissociation of Cl ₂ : potentials, transition moments, extinction coefficients, and Cl*/Cl branching ratio. <i>Journal of Chemical Physics</i> , 2004 , 120, 11549-56	3.9	27
36	The approach-induced I ₂ (E ₀ g ⁺ -MD ₀ u ⁺) transitions, M=He, Ar, I ₂ , N ₂ , CF ₄ . <i>Chemical Physics</i> , 2001 , 263, 459-470	2.3	26
35	TRAPP webserver: predicting protein binding site flexibility and detecting transient binding pockets. <i>Nucleic Acids Research</i> , 2017 , 45, W325-W330	20.1	25
34	Spectroscopic determination of the cold electron population in very low pressure ECR discharges in N ₂ /He mixtures. <i>Plasma Sources Science and Technology</i> , 2005 , 14, 109-128	3.5	25
33	Trends in adsorption of open-shell atoms and small molecular fragments on the Ag(111) surface. <i>Surface Science</i> , 2006 , 600, 5104-5113	1.8	22
32	Three steps to gold: mechanism of protein adsorption revealed by Brownian and molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 10191-200	3.6	22
31	Recent progress in molecular simulation methods for drug binding kinetics. <i>Current Opinion in Structural Biology</i> , 2020 , 64, 126-133	8.1	20
30	Perturbation Approaches for Exploring Protein Binding Site Flexibility to Predict Transient Binding Pockets. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 4100-13	6.4	20
29	Machine Learning Analysis of RAMD Trajectories to Decipher Molecular Determinants of Drug-Target Residence Times. <i>Frontiers in Molecular Biosciences</i> , 2019 , 6, 36	5.6	17
28	When the Label Matters: Adsorption of Labeled and Unlabeled Proteins on Charged Surfaces. <i>Nano Letters</i> , 2015 , 15, 7508-13	11.5	17
27	A workflow for exploring ligand dissociation from a macromolecule: Efficient random acceleration molecular dynamics simulation and interaction fingerprint analysis of ligand trajectories. <i>Journal of Chemical Physics</i> , 2020 , 153, 125102	3.9	17
26	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. <i>ACS Pharmacology and Translational Science</i> , 2021 , 4, 1079-1095	5.9	15
25	Druggability Assessment in TRAPP Using Machine Learning Approaches. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 1685-1699	6.1	14
24	HI photofragmentation revisited. Comment on "Probing excited electronic states using vibrationally mediated photolysis: Application to hydrogen iodide". <i>Journal of Physical Chemistry A</i> , 2005 , 109, 3094-6	2.8	14

23	The transition dipole moment function of the chlorine E0g+(3P2)B3D0u+ system. <i>Journal of Chemical Physics</i> , 1998 , 109, 10864-10872	3.9	14
22	Structure-kinetic relationship reveals the mechanism of selectivity of FAK inhibitors over PYK2. <i>Cell Chemical Biology</i> , 2021 , 28, 686-698.e7	8.2	13
21	Theoretical study of the CH2 + O photodissociation of formaldehyde adsorbed on the Ag(111) surface. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 18070-80	3.4	8
20	Configuration interaction study of the excited states of CO adsorbed on a Pt97 cluster. <i>Chemical Physics</i> , 2003 , 291, 115-124	2.3	7
19	Study of the covalent and triplet ionic-pairing states of the fluorine molecule with the MRDCI method. <i>Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)</i> , 2003 , 94, 170-178	0.7	7
18	A complete quantum mechanical study of chlorine photodissociation. <i>Journal of Chemical Physics</i> , 2012 , 136, 164310	3.9	6
17	Spectroscopic determination of cold electrons in electron cyclotron resonance discharges with highly charged ions. <i>Review of Scientific Instruments</i> , 1998 , 69, 1200-1202	1.7	6
16	Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems. <i>Journal of Computational Chemistry</i> , 2002 , 23, 943-9	3.5	6
15	Analysis of the bound-free emission spectra from the E(0+) and f(0+) ion-pair states of ClF to obtain potentials for the ion-pair and repulsive valence states. <i>Journal of Chemical Physics</i> , 1998 , 109, 1763-1771	3.9	6
14	Nonadiabatic effects in the lowest 0+(3P) ion-pair states of ClF. <i>Journal of Chemical Physics</i> , 2001 , 114, 3003-3009	3.9	5
13	Ligand unbinding mechanisms and kinetics for T4 lysozyme mutants from RAMD simulations. <i>Current Research in Structural Biology</i> , 2021 , 3, 106-111	2.8	5
12	Computational Approaches for Studying Drug Binding Kinetics. <i>Methods and Principles in Medicinal Chemistry</i> , 2015 , 211-235	0.4	4
11	The vibrationally mediated photodissociation of Cl2. <i>Journal of Chemical Physics</i> , 2012 , 137, 124310	3.9	4
10	Photodissociation of CH3Cl, C2H5Cl, and C6H5Cl on the Ag(111) surface: ab initio embedded cluster and configuration interaction study. <i>Journal of Chemical Physics</i> , 2010 , 132, 074707	3.9	4
9	Electric dipole moment function of the beta 1(3P2)toA 13Pi transition in ICl. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1999 , 32, 5325-5329	1.3	4
8	Electronic polarization effects in the photodissociation of Cl2. <i>Journal of Chemical Physics</i> , 2012 , 136, 164311	3.9	3
7	The lowest 1(3PJ) and 2(3P2) ion-pair states of ClF: Nonadiabatic effects and emission spectra. <i>Journal of Chemical Physics</i> , 2002 , 117, 628-635	3.9	3
6	Dynathor: Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase in a Phospholipid Bilayer 2016 , 255-264		2

5	Structure-Kinetic-Relationship Reveals the Mechanism of Selectivity of FAK Inhibitors Over PYK2. <i>SSRN Electronic Journal</i> ,	1	2
4	Theoretical Study of the Photoinduced C-H Bond Cleavage in Formaldehyde Adsorbed on the Ag(111) Surface. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 9914-9918	3.8	1
3	Brownian Dynamics Simulations of Proteins in the Presence of Surfaces: Long-Range Electrostatics and Mean-Field Hydrodynamics. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3510-3524	6.4	1
2	G Protein-Coupled Receptor-Ligand Dissociation Rates and Mechanisms from BAMD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6610-6623	6.4	1
1	Contact Map Fingerprints of Protein-Ligand Unbinding Trajectories Reveal Mechanisms Determining Residence Times Computed from Scaled Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 6522-6535	6.4	1