Daria B Kokh

List of Publications by Year in Descending Order

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	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. *ACS Pharmacology and Translational Science*, **2021**, 4, 1079-1095	5.9	15
57	Brownian Dynamics Simulations of Proteins in the Presence of Surfaces: Long-Range Electrostatics and Mean-Field Hydrodynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 3510-3524	6.4	1
56	Structure-kinetic relationship reveals the mechanism of selectivity of FAK inhibitors over PYK2. *Cell Chemical Biology*, **2021**, 28, 686-698.e7	8.2	13
55	Ligand unbinding mechanisms and kinetics for T4 lysozyme mutants from RAMD simulations. *Current Research in Structural Biology*, **2021**, 3, 106-111	2.8	5
54	G Protein-Coupled Receptor-Ligand Dissociation Rates and Mechanisms from RAMD Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6610-6623	6.4	1
53	Contact Map Fingerprints of Protein-Ligand Unbinding Trajectories Reveal Mechanisms Determining Residence Times Computed from Scaled Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2021**, 17, 6522-6535	6.4	1
52	Druggability Assessment in TRAPP Using Machine Learning Approaches. *Journal of Chemical Information and Modeling*, **2020**, 60, 1685-1699	6.1	14
51	A workflow for exploring ligand dissociation from a macromolecule: Efficient random acceleration molecular dynamics simulation and interaction fingerprint analysis of ligand trajectories. *Journal of Chemical Physics*, **2020**, 153, 125102	3.9	17
50	Recent progress in molecular simulation methods for drug binding kinetics. *Current Opinion in Structural Biology*, **2020**, 64, 126-133	8.1	20
49	Machine Learning Analysis of RAMD Trajectories to Decipher Molecular Determinants of Drug-Target Residence Times. *Frontiers in Molecular Biosciences*, **2019**, 6, 36	5.6	17
48	New approaches for computing ligand-receptor binding kinetics. *Current Opinion in Structural Biology*, **2018**, 49, 1-10	8.1	80
47	Estimation of Drug-Target Residence Times by Random Acceleration Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 3859-3869	6.4	95
46	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. *Drug Discovery Today*, **2017**, 22, 896-911	8.8	113
45	TRAPP webserver: predicting protein binding site flexibility and detecting transient binding pockets. *Nucleic Acids Research*, **2017**, 45, W325-W330	20.1	25
44	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. *Nature Communications*, **2017**, 8, 2276	17.4	101
43	Dynathor: Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase in a Phospholipid Bilayer **2016**, 255-264		2
42	Perturbation Approaches for Exploring Protein Binding Site Flexibility to Predict Transient Binding Pockets. *Journal of Chemical Theory and Computation*, **2016**, 12, 4100-13	6.4	20

41	Three steps to gold: mechanism of protein adsorption revealed by Brownian and molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2016**, 18, 10191-200	3.6	22
40	Modeling and simulation of protein-surface interactions: achievements and challenges. *Quarterly Reviews of Biophysics*, **2016**, 49, e4	7	112
39	Protein Binding Pocket Dynamics. *Accounts of Chemical Research*, **2016**, 49, 809-15	24.3	156
38	When the Label Matters: Adsorption of Labeled and Unlabeled Proteins on Charged Surfaces. *Nano Letters*, **2015**, 15, 7508-13	11.5	17
37	Computational Approaches for Studying Drug Binding Kinetics. *Methods and Principles in Medicinal Chemistry*, **2015**, 211-235	0.4	4
36	SDA 7: A modular and parallel implementation of the simulation of diffusional association software. *Journal of Computational Chemistry*, **2015**, 36, 1631-45	3.5	46
35	TRAPP: a tool for analysis of transient binding pockets in proteins. *Journal of Chemical Information and Modeling*, **2013**, 53, 1235-52	6.1	52
34	The vibrationally mediated photodissociation of Cl2. *Journal of Chemical Physics*, **2012**, 137, 124310	3.9	4
33	Electronic polarization effects in the photodissociation of Cl2. *Journal of Chemical Physics*, **2012**, 136, 164311	3.9	3
32	Docking of ubiquitin to gold nanoparticles. *ACS Nano*, **2012**, 6, 9863-78	16.7	112
31	A complete quantum mechanical study of chlorine photodissociation. *Journal of Chemical Physics*, **2012**, 136, 164310	3.9	6
30	Receptor flexibility in small-molecule docking calculations. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 298-314	7.9	38
29	Diffusion and association processes in biological systems: theory, computation and experiment. *BMC Biophysics*, **2011**, 4, 2	0	29
28	A quantitative, real-time assessment of binding of peptides and proteins to gold surfaces. *Chemistry - A European Journal*, **2011**, 17, 1327-36	4.8	34
27	Photodissociation of CH3Cl, C2H5Cl, and C6H5Cl on the Ag(111) surface: ab initio embedded cluster and configuration interaction study. *Journal of Chemical Physics*, **2010**, 132, 074707	3.9	4
26	ProMetCS: An Atomistic Force Field for Modeling Protein-Metal Surface Interactions in a Continuum Aqueous Solvent. *Journal of Chemical Theory and Computation*, **2010**, 6, 1753-68	6.4	51
25	Protein-surface interactions: challenging experiments and computations. *Journal of Molecular Recognition*, **2010**, 23, 259-62	2.6	33
24	High throughput in-silico screening against flexible protein receptors. *Journal of Cheminformatics*, **2010**, 2,	8.6	78

23	Flexible side chain models improve enrichment rates in in silico screening. *Journal of Medicinal Chemistry*, **2008**, 51, 5919-31	8.3	42
22	Theoretical Study of the Photoinduced C□H Bond Cleavage in Formaldehyde Adsorbed on the Ag(111) Surface. *Journal of Physical Chemistry C*, **2007**, 111, 9914-9918	3.8	1
21	Trends in adsorption of open-shell atoms and small molecular fragments on the Ag(111) surface. *Surface Science*, **2006**, 600, 5104-5113	1.8	22
20	HI photofragmentation revisited. Comment on "Probing excited electronic states using vibrationally mediated photolysis: Application to hydrogen iodide". *Journal of Physical Chemistry A*, **2005**, 109, 3094-6	2.8	14
19	Spectroscopic determination of the cold electron population in very low pressure ECR discharges in N2/He mixtures. *Plasma Sources Science and Technology*, **2005**, 14, 109-128	3.5	25
18	Theoretical study of the CH2 + O photodissociation of formaldehyde adsorbed on the Ag(111) surface. *Journal of Physical Chemistry B*, **2005**, 109, 18070-80	3.4	8
17	Theoretical study of the UV photodissociation of Cl2: potentials, transition moments, extinction coefficients, and Cl*/Cl branching ratio. *Journal of Chemical Physics*, **2004**, 120, 11549-56	3.9	27
16	Configuration interaction study of the excited states of CO adsorbed on a Pt97 cluster. *Chemical Physics*, **2003**, 291, 115-124	2.3	7
15	Study of the covalent and triplet ionic-pairing states of the fluorine molecule with the MRDCI method. *Optics and Spectroscopy (English Translation of Optika I Spektroskopiya)*, **2003**, 94, 170-178	0.7	7
14	Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems. *Journal of Computational Chemistry*, **2002**, 23, 943-9	3.5	6
13	The lowest 1(3PJ) and 2(3P2) ion-pair states of ClF: Nonadiabatic effects and emission spectra. *Journal of Chemical Physics*, **2002**, 117, 628-635	3.9	3
12	The approach-induced I2(E0g+-þMD0u+) transitions, M=He, Ar, I2, N2, CF4. *Chemical Physics*, **2001**, 263, 459-470	2.3	26
11	Nonadiabatic effects in the lowest 0+(3P) ion-pair states of ClF. *Journal of Chemical Physics*, **2001**, 114, 3003-3009	3.9	5
10	Ab initio study of spectroscopic and radiative characteristics of ion-pair states of the Cl2 molecule. *Journal of Chemical Physics*, **2001**, 115, 9298-9310	3.9	31
9	Relativistic configuration interaction study of the ClF molecule and its emission spectra from 0+ ion-pair states. *Journal of Chemical Physics*, **2000**, 112, 2274-2284	3.9	29
8	On the ultraviolet photofragmentation of hydrogen iodide. *Journal of Chemical Physics*, **2000**, 113, 6174-6185	3.9	59
7	Electric dipole moment function of the beta 1(3P2)toA 13Pi transition in ICl. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, 5325-5329	1.3	4
6	Spectroscopic determination of cold electrons in electron cyclotron resonance discharges with highly charged ions. *Review of Scientific Instruments*, **1998**, 69, 1200-1202	1.7	6

5	A comparative study of the electron distribution function in the positive columns in and /He dc glow discharges by optical spectroscopy and probes. *Plasma Sources Science and Technology*, **1998**, 7, 298-309	3.5	46
4	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. *Journal of Chemical Physics*, **1998**, 109, 1763-1771	3.9	6
3	The transition dipole moment function of the chlorine E0g+(3P2)B3□u+ system. *Journal of Chemical Physics*, **1998**, 109, 10864-10872	3.9	14
2	Absolute calibration of the efficiency of a VUV-monochromator/detector system in the range 110 - 450 nm. *Measurement Science and Technology*, **1997**, 8, 773-781	2	36
1	Structure-Kinetic-Relationship Reveals the Mechanism of Selectivity of FAK Inhibitors Over PYK2. *SSRN Electronic Journal*,	1	2