Daria B Kokh

List of Publications by Year
in descending order

60	2,500	172386	206029
papers	citations	29 h-index	48 g-index

64	64	64	3096
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Protein Binding Pocket Dynamics. Accounts of Chemical Research, 2016, 49, 809-815.	7.6	268
2	Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. Nature Communications, 2017, 8, 2276.	5.8	175
3	Estimation of Drug-Target Residence Times by Ï„-Random Acceleration Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3859-3869.	2.3	169
4	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. Drug Discovery Today, 2017, 22, 896-911.	3.2	165
5	Modeling and simulation of proteinâ€“surface interactions: achievements and challenges. Quarterly Reviews of Biophysics, 2016, 49, e4.	2.4	163
6	Docking of Ubiquitin to Gold Nanoparticles. ACS Nano, 2012, 6, 9863-9878.	7.3	131
7	New approaches for computing ligandâ€“receptor binding kinetics. Current Opinion in Structural Biology, 2018, 49, 1-10.	2.6	122
8	TRAPP: A Tool for Analysis of Transient Binding Pockets in Proteins. Journal of Chemical Information and Modeling, 2013, 53, 1235-1252.	2.5	72
9	<scp>SDA</scp> 7: A modular and parallel implementation of the simulation of diffusional association software. Journal of Computational Chemistry, 2015, 36, 1631-1645.	1.5	64
10	On the ultraviolet photofragmentation of hydrogen iodide. Journal of Chemical Physics, 2000, 113, 6174-6185.	1.2	61
11	Recent progress in molecular simulation methods for drug binding kinetics. Current Opinion in Structural Biology, 2020, 64, 126-133.	2.6	61
12	ProMetCS: An Atomistic Force Field for Modeling Proteinâ^'Metal Surface Interactions in a Continuum Aqueous Solvent. Journal of Chemical Theory and Computation, 2010, 6, 1753-1768.	2.3	58
13	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.	1.3	53
14	Flexible Side Chain Models Improve Enrichment Rates in In Silico Screening. Journal of Medicinal Chemistry, 2008, 51, 5919-5931.	2.9	49
15	Receptor flexibility in smallâ€molecule docking calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 298-314.	6.2	48
16	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.	1.2	45
17	TRAPP webserver: predicting protein binding site flexibility and detecting transient binding pockets. Nucleic Acids Research, 2017, 45, W325-W330.	6.5	44
18	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.	2.5	44

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19	Proteinâ€“surface interactions: challenging experiments and computations. Journal of Molecular Recognition, 2010, 23, 259-262.	1.1	41
20	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.	1.4	38
21	Perturbation Approaches for Exploring Protein Binding Site Flexibility to Predict Transient Binding Pockets. Journal of Chemical Theory and Computation, 2016, 12, 4100-4113.	2.3	38
22	Machine Learning Analysis of Ï„RAMD Trajectories to Decipher Molecular Determinants of Drug-Target Residence Times. Frontiers in Molecular Biosciences, 2019, 6, 36.	1.6	37
23	Structure-kinetic relationship reveals the mechanism of selectivity of FAK inhibitors over PYK2. Cell Chemical Biology, 2021, 28, 686-698.e7.	2.5	36
24	A Quantitative, Realâ€Time Assessment of Binding of Peptides and Proteins to Gold Surfaces. Chemistry - A European Journal, 2011, 17, 1327-1336.	1.7	35
25	Ab initio study of spectroscopic and radiative characteristics of ion-pair states of the Cl2 molecule. Journal of Chemical Physics, 2001, 115, 9298-9310.	1.2	32
26	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.	1.2	31
27	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.	1.3	31
28	Three steps to gold: mechanism of protein adsorption revealed by Brownian and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 10191-10200.	1.3	31
29	Ligand unbinding mechanisms and kinetics for T4 lysozyme mutants from Ï„RAMD simulations. Current Research in Structural Biology, 2021, 3, 106-111.	1.1	31
30	Diffusion and association processes in biological systems: theory, computation and experiment. BMC Biophysics, 2011, 4, 2.	4.4	30
31	Druggability Assessment in TRAPP Using Machine Learning Approaches. Journal of Chemical Information and Modeling, 2020, 60, 1685-1699.	2.5	29
32	The approach-induced I2( ) transitions, M=He, Ar, I2, N2, CF4. Chemical Physics, 2001, 263, 459-470.	0.9	27
33	Theoretical study of the UV photodissociation of Cl2: Potentials, transition moments, extinction coefficients, and Cl*/Cl branching ratio. Journal of Chemical Physics, 2004, 120, 11549-11556.	1.2	27
34	When the Label Matters: Adsorption of Labeled and Unlabeled Proteins on Charged Surfaces. Nano Letters, 2015, 15, 7508-7513.	4.5	24
35	Trends in adsorption of open-shell atoms and small molecular fragments on the Ag(111) surface. Surface Science, 2006, 600, 5104-5113.	0.8	23
36	G Protein-Coupled Receptorâ€“Ligand Dissociation Rates and Mechanisms from Ï„RAMD Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6610-6623.	2.3	21

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37	HI Photofragmentation Revisited. Comment on â€œProbing Excited Electronic States Using Vibrationally Mediated Photolysis:Â Application to Hydrogen Iodideâ€. Journal of Physical Chemistry A, 2005, 109, 3094-3096.	1.1	16
38	The transition dipole moment function of the chlorine E0g+(3P2)â^'B3Î0u+ system. Journal of Chemical Physics, 1998, 109, 10864-10872.	1.2	15
39	Contact Map Fingerprints of Proteinâ€“Ligand Unbinding Trajectories Reveal Mechanisms Determining Residence Times Computed from Scaled Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 6522-6535.	2.3	15
40	Configuration interaction study of the excited states of CO adsorbed on a Pt97 cluster. Chemical Physics, 2003, 291, 115-124.	0.9	8
41	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.	0.2	8
42	Theoretical Study of the CH2 + O Photodissociation of Formaldehyde Adsorbed on the Ag(111) Surface. Journal of Physical Chemistry B, 2005, 109, 18070-18080.	1.2	8
43	Analysis of the boundâ€“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.	1.2	7
44	A complete quantum mechanical study of chlorine photodissociation. Journal of Chemical Physics, 2012, 136, 164310.	1.2	7
45	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.	2.3	7
46	Spectroscopic determination of cold electrons in electron cyclotron resonance discharges with highly charged ions. Review of Scientific Instruments, 1998, 69, 1200-1202.	0.6	6
47	Nonadiabatic effects in the lowest 0+(3P) ion-pair states of ClF. Journal of Chemical Physics, 2001, 114, 3003-3009.	1.2	6
48	Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems. Journal of Computational Chemistry, 2002, 23, 943-949.	1.5	6
49	Graphene BioFET sensors for SARS-CoV-2 detection: a multiscale simulation approach. Nanoscale Advances, 0, , .	2.2	5
50	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.	0.6	4
51	Photodissociation of CH3Cl, C2H5Cl, and C6H5Cl on the Ag(111) surface:Ab initioembedded cluster and configuration interaction study. Journal of Chemical Physics, 2010, 132, 074707.	1.2	4
52	The vibrationally mediated photodissociation of Cl2. Journal of Chemical Physics, 2012, 137, 124310.	1.2	4
53	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.	1.2	3
54	Electronic polarization effects in the photodissociation of Cl2. Journal of Chemical Physics, 2012, 136, 164311.	1.2	3

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55	Dynathor: Dynamics of the Complex of Cytochrome P450 and Cytochrome P450 Reductase in a Phospholipid Bilayer. , 2016, , 255-264.		2
56	Structure-Kinetic-Relationship Reveals the Mechanism of Selectivity of FAK Inhibitors Over PYK2. SSRN Electronic Journal, 0, , .	0.4	2
57	Theoretical Study of the Photoinduced Câ^'H Bond Cleavage in Formaldehyde Adsorbed on the Ag(111) Surface. Journal of Physical Chemistry C, 2007, 111, 9914-9918.	1.5	1
58	Modeling of Protein Adsorption on a Metal Surface: Brownian Dynamics Simulations. Biophysical Journal, 2009, 96, 298a-299a.	0.2	1
59	High throughput in-silico screening against flexible protein receptors. Journal of Cheminformatics, 2010, 2, .	2.8	0
60	Comprehensive Characterization of Ligand Unbinding Mechanisms and Kinetics for T4 Lysozyme Mutants. Biophysical Journal, 2021, 120, 122a.	0.2	0