

# Fatemeh Keshavarz

## List of Publications by Year in descending order

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Version: 2024-02-01

21  
papers

160  
citations

1307366

7  
h-index

1199470

12  
g-index

22  
all docs

22  
docs citations

22  
times ranked

249  
citing authors

#	ARTICLE	IF	CITATIONS
1	Density Functional Theory-Based Adsorption Isotherms for Pure and Flue Gas Mixtures on Mg-MOF-74. Application in CO <sub>2</sub> Capture Swing Adsorption Processes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3945-3957.	1.5	38
2	Docking, molecular dynamics simulation studies, and structure-based QSAR model on cytochrome P450 2A6 inhibitors. <i>Structural Chemistry</i> , 2012, 23, 341-350.	1.0	20
3	Molecular-level understanding of highly selective heavy rare earth element uptake by organophosphorus modified MIL-101(Cr). <i>Chemical Engineering Journal</i> , 2022, 440, 135905.	6.6	12
4	Study on the interaction of three structurally related cationic Pt(II) complexes with human serum albumin: importance of binding affinity and denaturing properties. <i>Journal of the Iranian Chemical Society</i> , 2016, 13, 617-630.	1.2	10
5	Electrochemical Potential of the Metal Organic Framework MIL-101(Fe) as Cathode Material in Li-Ion Batteries. <i>Condensed Matter</i> , 2021, 6, 22.	0.8	10
6	Reaction Mechanisms Underlying Unfunctionalized Alkyl Nitrate Hydrolysis in Aqueous Aerosols. <i>ACS Earth and Space Chemistry</i> , 2021, 5, 210-225.	1.2	9
7	Molecular Origin of the Sign Preference of Ion- Induced Heterogeneous Nucleation in a Complex Ionic Liquid—Diethylene Glycol System. <i>Journal of Physical Chemistry C</i> , 2020, 124, 26944-26952.	1.5	8
8	New Particle Formation from the Vapor Phase: From Barrier-Controlled Nucleation to the Collisional Limit. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4593-4599.	2.1	8
9	A Structure-based QSAR and Docking Study on Imidazo[1,5-a][1,2,4]-triazolo[1,5-d][1,4]benzodiazepines as Selective GABA <sub>A</sub> Inverse Agonists. <i>Chemical Biology and Drug Design</i> , 2011, 78, 612-621.	1.5	7
10	Heterogeneous Nucleation of Butanol on NaCl: A Computational Study of Temperature, Humidity, Seed Charge, and Seed Size Effects. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3025-3036.	1.1	6
11	Probing the binding of thioTEPA to human serum albumin using spectroscopic and molecular simulation approaches. <i>Canadian Journal of Chemistry</i> , 2014, 92, 1066-1073.	0.6	5
12	Computational Study of the Effect of Mineral Dust on Secondary Organic Aerosol Formation by Accretion Reactions of Closed-Shell Organic Compounds. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9008-9018.	1.1	4
13	Spectroscopic and Molecular Dynamics Studies on Binding of Dimethylplatinum(II) Complex Drug to Human Serum Albumin. <i>Bulletin of the Chemical Society of Japan</i> , 2014, 87, 1094-1100.	2.0	3
14	A theoretical study on the dynamics of the gas phase reaction of NH <sub>2</sub> (2B1) with HO <sub>2</sub> (2A <sup>+</sup> ). <i>Journal of the Iranian Chemical Society</i> , 2016, 13, 1115-1124.	1.2	3
15	A single- and multireference study on CH <sub>2</sub> reaction with O <sub>2</sub> (). <i>International Journal of Chemical Kinetics</i> , 2019, 51, 161-177.	1.0	3
16	From Kinetics of OH Reaction with Glutamic Acid to Oxidative Damage to Proteins. <i>Journal of Physical Chemistry A</i> , 2019, 123, 429-442.	1.1	3
17	Molecular level insights into the direct health impacts of some organic aerosol components. <i>New Journal of Chemistry</i> , 2021, 45, 6709-6723.	1.4	3
18	Seed-Adsorbate Interactions as the Key of Heterogeneous Butanol and Diethylene Glycol Nucleation on Ammonium Bisulfate and Tetramethylammonium Bromide. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10527-10539.	1.1	3

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19	Anodic Activity of Hydrated and Anhydrous Iron (II) Oxalate in Li-Ion Batteries. Condensed Matter, 2022, 7, 8.	0.8	3
20	HER-2-based design of pertuzumab mimetic peptides. Molecular Simulation, 2015, 41, 1298-1307.	0.9	1
21	Chemical Kinetics Approves the Occurrence of C ( <sup>3</sup> P <sub>j</sub> ) Reaction with H <sub>2</sub> O. Journal of Physical Chemistry A, 2019, 123, 5877-5892.	1.1	1