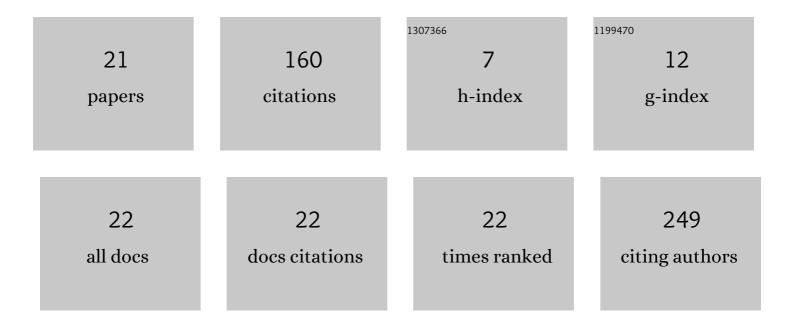
Fatemeh Keshavarz

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Density Functional Theory-Based Adsorption Isotherms for Pure and Flue Gas Mixtures on Mg-MOF-74. Application in CO ₂ Capture Swing Adsorption Processes. Journal of Physical Chemistry C, 2018, 122, 3945-3957.	1.5	38
2	Docking, molecular dynamics simulation studies, and structure-based QSAR model on cytochrome P450 2A6 inhibitors. Structural Chemistry, 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). Chemical Engineering Journal, 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. Journal of the Iranian Chemical Society, 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. Condensed Matter, 2021, 6, 22.	0.8	10
6	Reaction Mechanisms Underlying Unfunctionalized Alkyl Nitrate Hydrolysis in Aqueous Aerosols. ACS Earth and Space Chemistry, 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. Journal of Physical Chemistry C, 2020, 124, 26944-26952.	1.5	8
8	New Particle Formation from the Vapor Phase: From Barrier-Controlled Nucleation to the Collisional Limit. Journal of Physical Chemistry Letters, 2021, 12, 4593-4599.	2.1	8
9	A Structureâ€based QSAR and Docking Study on Imidazo[1,5â€a][1,2,4]â€triazolo[1,5â€d][1,4,]benzodiazepine Selective GABA _A α5 Inverse Agonists. Chemical Biology and Drug Design, 2011, 78, 612-621.	s as 1.5	7
10	Heterogeneous Nucleation of Butanol on NaCl: A Computational Study of Temperature, Humidity, Seed Charge, and Seed Size Effects. Journal of Physical Chemistry A, 2021, 125, 3025-3036.	1.1	6
11	Probing the binding of thioTEPA to human serum albumin using spectroscopic and molecular simulation approaches. Canadian Journal of Chemistry, 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. Journal of Physical Chemistry A, 2019, 123, 9008-9018.	1.1	4
13	Spectroscopic and Molecular Dynamics Studies on Binding of Dimethylplatinum(II) Complex Drug to Human Serum Albumin. Bulletin of the Chemical Society of Japan, 2014, 87, 1094-1100.	2.0	3
14	A theoretical study on the dynamics of the gas phase reaction of NH2(2B1) with HO2(2Aâ \in ³). Journal of the Iranian Chemical Society, 2016, 13, 1115-1124.	1.2	3
15	A single―and multireference study on CH (X ² Î) reaction with O ₂ (). International Journal of Chemical Kinetics, 2019, 51, 161-177.	1.0	3
16	From Kinetics of OH Reaction with Glutamic Acid to Oxidative Damage to Proteins. Journal of Physical Chemistry A, 2019, 123, 429-442.	1.1	3
17	Molecular level insights into the direct health impacts of some organic aerosol components. New Journal of Chemistry, 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. Journal of Physical Chemistry A, 2020, 124, 10527-10539.	1.1	3

#	Article	IF	CITATIONS
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 (³ P _{<i>j</i>}) Reaction with H ₂ O. Journal of Physical Chemistry A, 2019, 123, 5877-5892.	1.1	1