Peng Li

List of Publications by Year
in descending order

23	942	933447 10	713466 21
papers	citations	h-index	g-index

23	23	23	796
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Two-photon Raman transition channels of NaCs predicted from ab initio calculations. Physical Review A, 2022, 105, .	2.5	0
2	Hyperfine structure of the NaCs b³Î₂ state near the dissociation limit 3S_{1/2} + 6P_{3/2} observed with ultracold atomic photoassociation. Physical Chemistry Chemical Physics, 2020, 22, 3809-3816.	2.8	6
3	Actinyl-Carboxylate Complexes [AnO₂(COOH)_n(H₂O)_m]^{2â€“n} (An = U, Np, Pu, and Am; n = 1â€“3; m = 0, 2, 4; 2n + m = 6): Electronic Structures, Interaction Features, and the Potential to Adsorbents toward Cs Ion. ACS Omega, 2020, 5, 31074-31083.	3.5	2
4	Reaction mechanisms and topological analyses for the C H activation of ethylene by uranium atom using density functional theory. Computational and Theoretical Chemistry, 2020, 1190, 113022.	2.5	1
5	Ab initio predictions for the reaction mechanism and orbital topological properties of the formation of Neptunimine, Plutonimine, and its side products. Journal of Molecular Modeling, 2020, 26, 163.	1.8	1
6	Reaction mechanism of synthetic thorium sulfides: theoretical calculation study. Journal of Molecular Modeling, 2020, 26, 123.	1.8	0
7	The formation mechanism of uranium and thorium hydride phosphorus: a systematically theoretical study. RSC Advances, 2019, 9, 17119-17128.	3.6	3
8	Organic Compounds of Actinyls: Systematic Computational Assessment of Structural and Topological Properties in [AnO₂(C₂O₄)_n]^{(2nâ^2)â€“} (An) Tj ETQq0 0 0 rgBT /Ove	4.0	11
9	Successful Decontamination of ⁹⁹TcO₄^{â^’} in Groundwater at Legacy Nuclear Sites by a Cationic Metalâ€Organic Framework with Hydrophobic Pockets. Angewandte Chemie - International Edition, 2019, 58, 4968-4972.	13.8	177
10	Actinide Endohedral and Exohedral Cubic Siloxanes: An(IV)@(HSiO_{1.5})₈ and An(IV)&(RSiO_{1.5})₈ (An = U, Np, Pu; R = H, Cl, OH). European Journal of Inorganic Chemistry, 2019, 2019, 4660-4667.	2.0	2
11	Can water continuously oxidize the PuO molecule? Mechanisms, topological analysis and rate constant calculations. RSC Advances, 2018, 8, 4295-4303.	3.6	4
12	99TcO4â^’ remediation by a cationic polymeric network. Nature Communications, 2018, 9, 3007.	12.8	234
13	Systematic analysis of structural and topological properties: new insights into PuO2(H2O)n2+ (n =) Tj ETQq1 1 0.784314 rgBT /Overlo	3.6	7
14	Identifying the Recognition Site for Selective Trapping of ⁹⁹TcO₄^{â€“} in a Hydrolytically Stable and Radiation Resistant Cationic Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 14873-14876.	13.7	386
15	xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>c</mml:mi><mml:mspace width="0.16em" /><mml:mmultiscripts><mml:mi mathvariant="normal">Î£</mml:mi><mml:none /><mml:mo>+</mml:mo><mml:mprescripts /><mml:none /><mml:mn>3</mml:mn></mml:mmultiscripts></mml:mrow></mml:math>state below the dissociation limit</mml:math>	2.5	17
16	Gasâ€phase ammonia activation by Th, Th⁺, and Th²⁺: Reaction mechanisms, bonding analysis, and rate constant calculations. International Journal of Quantum Chemistry, 2015, 115, 6-18.	2.0	15
17	Systematic analysis of structural and spectroscopic properties of neptunimine (HN=NpH2) and plutonimine (HN=PuH2). Journal of Molecular Modeling, 2015, 21, 316.	1.8	4
18	Mechanistic aspects of the reaction of uranium atom with H2O in the gas phase. Journal of Radioanalytical and Nuclear Chemistry, 2015, 304, 489-499.	1.5	9

#	Article	IF	Citations
19	Reaction of Np atom with H2O in the gas phase: reaction mechanisms and ab initio molecular dynamics study. Journal of Molecular Modeling, 2014, 20, 2466.	1.8	3
20	Gasâ€phase water activation by Th atom: Reaction mechanisms and topological analysis. International Journal of Quantum Chemistry, 2014, 114, 760-768.	2.0	14
21	Water Oï£¿H Bond Activation by Gasâ€Phase Plutonium Atoms: Reaction Mechanisms and Ab Initio Molecular Dynamics Study. ChemPhysChem, 2014, 15, 3078-3088.	2.1	16
22	Investigation of the reactions of U, U⁺and U²⁺with ammonia: mechanisms and topological analysis. RSC Advances, 2014, 4, 29806.	3.6	20
23	Ab Initio Molecular Dynamics Study of the Reaction of U⁺ and U²⁺ with H₂O in the Gas Phase: Direct Classical Trajectory Calculations. Journal of Physical Chemistry A, 2013, 117, 3761-3770.	2.5	10