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List of Publications by Year
in descending order

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48 papers	3,059 citations	318942 23 h-index	232693 48 g-index
49 all docs	49 docs citations	49 times ranked	5521 citing authors

#	Article	IF	Citations
1	Time-Dependent Density Functional Theory Study of Copper(II) Oxo Active Sites for Methane-to-Methanol Conversion in Zeolites. Inorganic Chemistry, 2021, 60, 1149-1159.	1.9	10
2	Copper-Oxo Active Sites in the 8MR of Zeolite Mordenite: DFT Investigation of the Impact of Acid Sites on Methanol Yield and Selectivity. Journal of Physical Chemistry C, 2021, 125, 6684-6693.	1.5	5
3	Methane Câ€“H Activation by [Cu₂O]²⁺ and [Cu₃O₃]²⁺ in Copper-Exchanged Zeolites: Computational Analysis of Redox Chemistry and X-ray Absorption Spectroscopy. Inorganic Chemistry, 2021, 60, 6218-6227.	1.9	5
4	Methane Overâ€Oxidation by Extraâ€Framework Copperâ€Oxo Active Sites of Copperâ€Exchanged Zeolites: Crucial Role of Traps for the Separated Methyl Group. ChemPhysChem, 2021, 22, 1101-1109.	1.0	7
5	Copper-Oxo Active Sites for Methane Câ€“H Activation in Zeolites: Molecular Understanding of Impact of Methane Hydroxylation on UVâ€“Vis Spectra. Inorganic Chemistry, 2021, 60, 8489-8499.	1.9	11
6	DFT Analysis of Methane Câˆ’H Activation and Overâ€Oxidation by [Cu₂O]²⁺ and [Cu₂O₂]²⁺ Sites in Zeolite Mordenite: Intraâ€versus Interâ€site Overâ€Oxidation. ChemPhysChem, 2021, 22, 2517-2525.	1.0	2
7	Heterometallic [Cuâ€“Oâ€“M]²⁺active sites for methane Câ€“H activation in zeolites: stability, reactivity, formation mechanism and relationship to other active sites. Catalysis Science and Technology, 2021, 11, 5671-5683.	2.1	3
8	2D-IR studies of cyanamides (NCN) as spectroscopic reporters of dynamics in biomolecules: Uncovering the origin of mysterious peaks. Journal of Chemical Physics, 2020, 152, 074201.	1.2	7
9	Activating Water and Hydrogen by Ligand-Modified Uranium and Neptunium Complexes: A Density Functional Theory Study. Inorganic Chemistry, 2020, 59, 3102-3109.	1.9	2
10	Pyrazole, Imidazole, and Isoindolone Dipyrrinone Analogues: pH-Dependent Fluorophores That Red-Shift Emission Frequencies in a Basic Solution. Journal of Organic Chemistry, 2019, 84, 11856-11862.	1.7	6
11	Ground-state actinide chemistry with scalar-relativistic multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2019, 151, 134102.	1.2	12
12	Nitrogen Reduction by Multimetallic trans-Uranium Actinide Complexes: A Theoretical Comparison of Np and Pu to U. Inorganic Chemistry, 2019, 58, 6731-6741.	1.9	7
13	Correction to â€œTuning Zr₆ Metal-Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalystsâ€• ACS Catalysis, 2018, 8, 2364-2364.	5.5	3
14	Performance of Density Functional Theory for Predicting Methane-to-Methanol Conversion by a Tri-Copper Complex. Journal of Physical Chemistry C, 2018, 122, 1024-1036.	1.5	23
15	Performance of density functional theory for describing heteroâ€metallic activeâ€site motifs for methaneâ€toâ€methanol conversion in metalâ€exchanged zeolites. Journal of Computational Chemistry, 2018, 39, 2667-2678.	1.5	8
16	Predicting Bond Dissociation Energies of Transition-Metal Compounds by Multiconfiguration Pair-Density Functional Theory and Second-Order Perturbation Theory Based on Correlated Participating Orbitals and Separated Pairs. Journal of Chemical Theory and Computation, 2017, 13, 616-626.	2.3	47
17	What Is the Preferred Conformation of Phosphatidylserineâ€“Copper(II) Complexes? A Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry B, 2016, 120, 12883-12889.	1.2	13
18	Charge Transport in 4 nm Molecular Wires with Interrupted Conjugation: Combined Experimental and Computational Evidence for Thermally Assisted Polaron Tunneling. ACS Nano, 2016, 10, 4372-4383.	7.3	56

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19	Separated-pair approximation and separated-pair pair-density functional theory. Chemical Science, 2016, 7, 2399-2413.	3.7	47
20	Structure and Reactivity of X-ray Amorphous Uranyl Peroxide, U₂O₇. Inorganic Chemistry, 2016, 55, 3541-3546.	1.9	50
21	Tuning Zr₆ Metalâ€“Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalysts. ACS Catalysis, 2016, 6, 235-247.	5.5	150
22	Metalâ€“Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000- and UiO-66-Supported Iridium Complexes. Journal of the American Chemical Society, 2015, 137, 7391-7396.	6.6	228
23	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
24	Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metalâ€“Metal-Bonded Complexes?. Journal of Chemical Theory and Computation, 2015, 11, 4093-4101.	2.3	20
25	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	3.7	45
26	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
27	Investigation of the Electronic Ground States for a Reduced Pyridine(diimine) Uranium Series: Evidence for a Ligand Tetraanion Stabilized by a Uranium Dimer. Journal of the American Chemical Society, 2015, 137, 4690-4700.	6.6	62
28	Probing the mechanism of CO₂ capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457.	1.3	43
29	Length-Dependent Nanotransport and Charge Hopping Bottlenecks in Long Thiophene-Containing Ï€-Conjugated Molecular Wires. Journal of the American Chemical Society, 2015, 137, 15732-15741.	6.6	76
30	Preferential Location of Germanium in the UTL and IPC-2a Zeolites. Journal of Physical Chemistry C, 2014, 118, 26939-26946.	1.5	17
31	UO₂²⁺ Uptake by Proteins: Understanding the Binding Features of the Super Uranyl Binding Protein and Design of a Protein with Higher Affinity. Journal of the American Chemical Society, 2014, 136, 17484-17494.	6.6	74
32	Harnessing redox activity for the formation of uranium tris(imido) compounds. Nature Chemistry, 2014, 6, 919-926.	6.6	145
33	Oxo-Exchange of Gas-Phase Uranyl, Neptunyl, and Plutonyl with Water and Methanol. Inorganic Chemistry, 2014, 53, 2163-2170.	1.9	19
34	Investigation of the Electronic Structure of Mono(1,1â€²-Diamidoferrocene) Uranium(IV) Complexes. Organometallics, 2013, 32, 6012-6021.	1.1	27
35	Coordination and Hydrolysis of Plutonium Ions in Aqueous Solution Using Carâ€“Parrinello Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry A, 2013, 117, 12256-12267.	1.1	35
36	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8

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37	Oxo-Functionalization and Reduction of the Uranyl Ion through Lanthanide-Element Bond Homolysis: Synthetic, Structural, and Bonding Analysis of a Series of Singly Reduced Uranylâ€“Rare Earth 5f¹-4fⁿ Complexes. Journal of the American Chemical Society, 2013, 135, 3841-3854.	6.6	107
38	Theoretical Study of Structural, Spectroscopic and Reaction Properties of trans-bis(imido) Uranium(VI) Complexes. Inorganic Chemistry, 2013, 52, 9143-9152.	1.9	11
39	DFT Study of Uranyl Peroxo Complexes with H₂O, F^{â€“}, OH^{â€“}, CO₃²⁻, and NO₃^{â€“}. Inorganic Chemistry, 2013, 52, 5590-5602.	1.9	40
40	DFT Study of Oxo-Functionalized Pentavalent Dioxouranium Complexes: Structure, Bonding, Ligand Exchange, Dimerization, and U(V)/U(IV) Reduction of OUOH and OUOSiH3Complexes. Inorganic Chemistry, 2013, 52, 245-257.	1.9	8
41	Strongly coupled binuclear uraniumâ€“oxo complexes from uranyl oxo rearrangement and reductive silylation. Nature Chemistry, 2012, 4, 221-227.	6.6	149
42	Theoretical Study of the Reduction of Uranium(VI) Aquo Complexes on Titania Particles and by Alcohols. Chemistry - A European Journal, 2012, 18, 7117-7127.	1.7	29
43	Adsorption of Uranyl Species onto the Rutile (110) Surface: A Periodic DFT Study. Chemistry - A European Journal, 2012, 18, 1458-1466.	1.7	37
44	Structures, spectroscopic properties and redox potentials of quaterpyridyl Ru(ii) photosensitizer and its derivatives for solar energy cell: a density functional study. Physical Chemistry Chemical Physics, 2011, 13, 14481.	1.3	19
45	QM and QM/MM Studies of Uranyl Fluorides in the Gas and Aqueous Phases and in the Hydrophobic Cavities of Tetrabrachion. Inorganic Chemistry, 2011, 50, 3141-3152.	1.9	22
46	Theoretical Study of the Structural Properties of Plutonium(IV) and (VI) Complexes. Journal of Physical Chemistry A, 2011, 115, 14110-14119.	1.1	35
47	Performance of Relativistic Effective Core Potentials in DFT Calculations on Actinide Compounds. Journal of Physical Chemistry A, 2010, 114, 1957-1963.	1.1	60
48	F 1s spectroscopy and ionic fragmentation of trifluoropropyne. Canadian Journal of Chemistry, 2008, 86, 761-768.	0.6	2