Andrew Kerridge

List of Publications by Year
in descending order

53	1,985	236925 25	254184 43
papers	citations	h-index	g-index

62	62	62	1941
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Thin Films: A New Type of Magnetic Switch. Advanced Materials, 2007, 19, 3618-3622.	21.0	133
2	The inverse-trans-influence in tetravalent lanthanide and actinide bis(carbene) complexes. Nature Communications, 2017, 8, 14137.	12.8	128
3	Energy-Degeneracy-Driven Covalency in Actinide Bonding. Journal of the American Chemical Society, 2018, 140, 17977-17984.	13.7	108
4	Quantification of f-element covalency through analysis of the electron density: insights from simulation. Chemical Communications, 2017, 53, 6685-6695.	4.1	102
5	Actinide covalency measured by pulsed electron paramagnetic resonance spectroscopy. Nature Chemistry, 2017, 9, 578-583.	13.6	102
6	Oxidation state and covalency in f-element metallocenes (M = Ce, Th, Pu): a combined CASSCF and topological study. Dalton Transactions, 2013, 42, 16428.	3.3	90
7	Emergence of comparable covalency in isostructural cerium(<scp>iv</scp>)â€“ and uranium(<scp>iv</scp>)â€“carbon multiple bonds. Chemical Science, 2016, 7, 3286-3297.	7.4	90
8	f-Orbital covalency in the actinocenes (An = Thâ€“Cm): multiconfigurational studies and topological analysis. RSC Advances, 2014, 4, 12078-12086.	3.6	78
9	Is Cerocene Really a Ce(III) Compound? All-Electron Spinâˆ'Orbit Coupled CASPT2 Calculations on M(Î·⁸-C₈H₈)₂(M = Th, Pa, Ce). Journal of Physical Chemistry A, 2009, 113, 2896-2905.	2.5	72
10	Emission spectroscopy of uranium(iv) compounds: a combined synthetic, spectroscopic and computational study. RSC Advances, 2013, 3, 4350.	3.6	57
11	Uâ€“O_{yl} Stretching Vibrations as a Quantitative Measure of the Equatorial Bond Covalency in Uranyl Complexes: A Quantum-Chemical Investigation. Inorganic Chemistry, 2016, 55, 573-583.	4.0	53
12	Water Adsorption on AnO₂ {111}, {110}, and {100} Surfaces (An = U and Pu): A Density Functional Theory + U Study. Journal of Physical Chemistry C, 2017, 121, 1675-1682.	3.1	48
13	Why Do Some Molecules Form Hydrates or Solvates?. Crystal Growth and Design, 2018, 18, 1903-1908.	3.0	47
14	Oxygen Vacancy Formation and Water Adsorption on Reduced AnO₂{111}, {110}, and {100} Surfaces (An = U, Pu): A Computational Study. Journal of Physical Chemistry C, 2018, 122, 7149-7165.	3.1	45
15	Importance of Quantum Tunneling in Vacancy-Hydrogen Complexes in Diamond. Physical Review Letters, 2005, 95, 105502.	7.8	42
16	Are the Ground States of the Later Actinocenes Multiconfigurational? All-Electron Spinâˆ'Orbit Coupled CASPT2 Calculations on An(Î·⁸-C₈H₈)₂(An =) Tj ETQq1 1 0 rgBT /Overlock	2.5	41
17	Topological Study of Bonding in Aquo and Bis(triazinyl)pyridine Complexes of Trivalent Lanthanides and Actinides: Does Covalency Imply Stability?. Inorganic Chemistry, 2016, 55, 10034-10042.	4.0	41
18	Concomitant Carboxylate and Oxalate Formation From the Activation of CO₂ by a Thorium(III) Complex. Chemistry - A European Journal, 2016, 22, 17976-17979.	3.3	39

#	Article	IF	Citations
19	Structure-dependent exchange in the organic magnets Cu(II)Pc and Mn(II)Pc. Physical Review B, 2008, 77, .	3.2	38
20	Dithio- and Diselenophosphinate Thorium(IV) and Uranium(IV) Complexes: Molecular and Electronic Structures, Spectroscopy, and Transmetalation Reactivity. Inorganic Chemistry, 2015, 54, 11625-11636.	4.0	35
21	Optical excitation of MgO nanoparticles; a computational perspective. Physical Chemistry Chemical Physics, 2014, 16, 22052-22061.	2.8	33
22	Assessing Covalency in Cerium and Uranium Hexachlorides: A Correlated Wavefunction and Density Functional Theory Study. Inorganics, 2015, 3, 482-499.	2.7	33
23	Electronic structure of bulk AnO 2 (AnÂ=ÂU, Np, Pu) and water adsorption on the (111) and (110) surfaces of UO 2 and PuO 2 from hybrid density functional theory within the periodic electrostatic embedded cluster method. Journal of Nuclear Materials, 2016, 482, 124-134.	2.7	30
24	White phosphorus activation by a Th(<scp>iii</scp>) complex. Dalton Transactions, 2016, 45, 2390-2393.	3.3	30
25	Yttrium Complexes of Arsine, Arsenide, and Arsinidene Ligands. Angewandte Chemie - International Edition, 2015, 54, 4255-4258.	13.8	28
26	Double Reduction of 4,4â€²â€Bipyridine and Reductive Coupling of Pyridine by Two Thorium(III) Singleâ€Electron Transfers. Chemistry - A European Journal, 2017, 23, 2290-2293.	3.3	26
27	Solubility prediction from first principles: a density of states approach. Physical Chemistry Chemical Physics, 2018, 20, 20981-20987.	2.8	26
28	Assessing covalency in equatorial Uâ€“N bonds: density based measures of bonding in BTP and isoamethyrin complexes of uranyl. Physical Chemistry Chemical Physics, 2016, 18, 16830-16839.	2.8	24
29	Coordination Chemistry and QTAIM Analysis of Homoleptic Dithiocarbamate Complexes, M(S₂CNⁱPr₂)₄ (M = Ti, Zr, Hf, Th, U, Np). Inorganic Chemistry, 2018, 57, 10518-10524.	4.0	24
30	All-electron CASPT2 study of Ce(Î·8â€“C8H6)2. Comptes Rendus Chimie, 2010, 13, 853-859.	0.5	23
31	Probing hydrogen and halogen-oxo interactions in uranyl coordination polymers: a combined crystallographic and computational study. CrystEngComm, 2018, 20, 4916-4925.	2.6	23
32	A mystery solved? Photoelectron spectroscopic and quantum chemical studies of the ion states of CeCp3+. Dalton Transactions, 2009, , 5943.	3.3	21
33	Quantum behaviour of hydrogen and muonium in vacancy-containing complexes in diamond. Journal of Physics Condensed Matter, 2004, 16, 8743-8751.	1.8	19
34	Decomposition of d- and f-Shell Contributions to Uranium Bonding from the Quantum Theory of Atoms in Molecules: Application to Uranium and Uranyl Halides. Inorganics, 2018, 6, 88.	2.7	19
35	Neptunyl(<scp>vi</scp>) centred visible LMCT emission directly observable in the presence of uranyl(<scp>vi</scp>). Chemical Communications, 2015, 51, 5402-5405.	4.1	18
36	Factors affecting the nucleus-independent chemical shift in NMR studies of microporous carbon electrode materials. Energy Storage Materials, 2019, 21, 335-346.	18.0	18

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37	Quantum Chemical Studies of the Hydration of Sr²⁺ in Vacuum and Aqueous Solution. Chemistry - A European Journal, 2011, 17, 5060-5067.	3.3	17
38	A RASSCF study of free base, magnesium and zinc porphyrins: accuracy versus efficiency. Physical Chemistry Chemical Physics, 2013, 15, 2197.	2.8	17
39	How to Bend the Uranyl Cation via Crystal Engineering. Inorganic Chemistry, 2018, 57, 2714-2723.	4.0	17
40	Elucidation of the inverse trans influence in uranyl and its imido and carbene analogues via quantum chemical simulation. Chemical Communications, 2018, 54, 9761-9764.	4.1	16
41	Systematic Investigation of the Molecular and Electronic Structure of Thorium and Uranium Phosphorus and Arsenic Complexes. Inorganic Chemistry, 2021, 60, 10614-10630.	4.0	15
42	Should environmental effects be included when performing QTAIM calculations on actinide systems? A comparison of QTAIM metrics for Cs2UO2Cl4, U(Se2PPh2)4 and Np(Se2PPh2)4 in gas phase, COSMO and PEECM. Polyhedron, 2016, 116, 57-63.	2.2	14
43	Unravelling the electronic structure and dynamics of an isolated molecular rotary motor in the gas-phase. Chemical Science, 2017, 8, 6141-6148.	7.4	13
44	Ligand size dependence of Uâ€“N and Uâ€“O bond character in a series of uranyl hexaphyrin complexes: quantum chemical simulation and density based analysis. Physical Chemistry Chemical Physics, 2017, 19, 7546-7559.	2.8	10
45	The importance of second shell effects in the simulation of hydrated Sr2+ hydroxide complexes. Dalton Transactions, 2015, 44, 11572-11581.	3.3	9
46	The coordination of Sr2+ by hydroxide: a density functional theoretical study. Dalton Transactions, 2011, 40, 11258.	3.3	8
47	Electron dynamics in quantum gate operation. Journal of Physics Condensed Matter, 2007, 19, 282201.	1.8	7
48	Ionic adsorption on the brucite (0001) surface: A periodic electrostatic embedded cluster method study. Journal of Chemical Physics, 2016, 145, 204708.	3.0	7
49	Structural, spectroscopic, and computational evaluations of cationâ€“cation and halogen bonding interactions in heterometallic uranyl hybrid materials. Inorganic Chemistry Frontiers, 2021, 8, 1128-1141.	6.0	7
50	Does Reduction-Induced Isomerization of a Uranium(III) Aryl Complex Proceed via Câ€“H Oxidative Addition and Reductive Elimination across the Uranium(II/IV) Redox Couple?. Inorganic Chemistry, 2022, 61, 8955-8965.	4.0	7
51	Ab initio molecular dynamics studies of hydroxide coordination of alkaline earth metals and uranyl. Physical Chemistry Chemical Physics, 2019, 21, 13809-13820.	2.8	6
52	Time dependent quantum simulations of two-qubit gates based on donor states in silicon. Journal of Physics Condensed Matter, 2006, 18, S767-S776.	1.8	5
53	Photoluminescence of Pentavalent Uranyl Amide Complexes. Journal of the American Chemical Society, 2021, 143, 13184-13194.	13.7	5