Nikolas Kaltsoyannis

List of Publications by Year
in descending order

203	8,511	38660 50	58464 82
papers	citations	h-index	g-index

219	219	219	5010
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational study of the energy landscape of water on the ThO2 {111} surface. Journal of Nuclear Materials, 2022, 559, 153476.	1.3	4
2	Hybrid functional/embedded cluster study of uranium and actinide (actinideÂ=ÂNp, Pu, Am or Cm) mixed dioxides bulk and {110} surfaces. Journal of Nuclear Materials, 2022, 560, 153490.	1.3	2
3	Accommodation of helium in PuO_{2Â±x} and the role of americium. Physical Chemistry Chemical Physics, 2022, 24, 8245-8250.	1.3	3
4	Covalency in AnCl₂ (An = Thâ€“No). Dalton Transactions, 2022, 51, 5929-5937.	1.6	0
5	Reply to: [{Th(C8H8)Cl2}3]2â^' is stable but not aromatic. Nature, 2022, 603, E21-E22.	13.7	9
6	Uraniumâ€“nitride chemistry: uraniumâ€“uranium electronic communication mediated by nitride bridges. Dalton Transactions, 2022, 51, 8855-8864.	1.6	4
7	Diffusion of krypton and xenon in uranium mononitride; a Density Functional Theory Study. Journal of Nuclear Materials, 2022, 566, 153803.	1.3	2
8	DFT + U Study of Uranium Dioxide and Plutonium Dioxide with Occupation Matrix Control. Journal of Physical Chemistry C, 2022, 126, 11426-11435.	1.5	13
9	Contrasting behaviour under pressure reveals the reasons for pyramidalization in tris(amido)uranium(III) and tris(arylthiolate) uranium(III) molecules. Nature Communications, 2022, 13, .	5.8	7
10	Computational study of the substitution of early actinides and Ce into zirconolite. Journal of Nuclear Materials, 2021, 543, 152525.	1.3	4
11	Embedded Cluster Study of the Co-Adsorption of HCl and H2O on PuO2 Surfaces. Journal of Nuclear Materials, 2021, 545, 152623.	1.3	4
12	DFTÂ+ÂU study of U1-An O2- (AnÂ=ÂNp, Pu, Am and Cm) {1 1 1}, {1 1 0} and {1 0 0} surfaces. Applied Surface Science, 2021, 537, 147972.	3.1	4
13	Covalency in AnCl₃ (An = Thâ€“No). Dalton Transactions, 2021, 50, 1478-1485.	1.6	17
14	High coordination number actinide-noble gas complexes; a computational study. Physical Chemistry Chemical Physics, 2021, 23, 4167-4177.	1.3	3
15	Synthesis, structure, and reactivity of uranium(<scp>vi</scp>) nitrides. Chemical Science, 2021, 12, 8096-8104.	3.7	18
16	²⁹Si NMR Spectroscopy as a Probe of s- and f-Block Metal(II)â€“Silanide Bond Covalency. Journal of the American Chemical Society, 2021, 143, 9813-9824.	6.6	11
17	A crystalline tri-thorium cluster with Ïƒ-aromatic metalâ€“metal bonding. Nature, 2021, 598, 72-75.	13.7	52
18	Exceptional uranium(VI)-nitride triple bond covalency from 15N nuclear magnetic resonance spectroscopy and quantum chemical analysis. Nature Communications, 2021, 12, 5649.	5.8	26

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19	Incorporation of Kr and Xe in Uranium Mononitride: A Density Functional Theory Study. Journal of Physical Chemistry C, 2021, 125, 26999-27008.	1.5	10
20	Crystallinity-Modulated Co_{2â€“x}V_xO₄ Nanoplates for Efficient Electrochemical Water Oxidation. ACS Catalysis, 2021, 11, 14884-14891.	5.5	23
21	Formation of a U(VI)â€“Persulfide Complex during Environmentally Relevant Sulfidation of Iron (Oxyhydr)oxides. Environmental Science & Technology, 2020, 54, 129-136.	4.6	17
22	Formation of Mn hydrides from bis(trimethylsilylmethyl) Mn(II): A DFT study. Polyhedron, 2020, 178, 114355.	1.0	0
23	Polarised covalent thorium(<scp>iv</scp>)â€“ and uranium(<scp>iv</scp>)â€“silicon bonds. Chemical Communications, 2020, 56, 12620-12623.	2.2	11
24	The ditungsten decacarbonyl dianion. Dalton Transactions, 2020, 49, 9330-9335.	1.6	3
25	Adsorption of U(VI) on Stoichiometric and Oxidised Mackinawite: a DFT Study. Environmental Science & Technology, 2020, 54, 6792-6799.	4.6	14
26	Synthesis of a â€œMaskedâ€•Terminal Zinc Sulfide and Its Reactivity with BrÃ¸nsted and Lewis Acids. Angewandte Chemie - International Edition, 2020, 59, 8947-8951.	7.2	8
27	Computational Study of Plutoniumâ€“Americium Mixed Oxides (Pu0.92Am0.08O2â€“x); Water Adsorption on {111}, {110}, and {100} Surfaces. Journal of Physical Chemistry C, 2020, 124, 6646-6658.	1.5	10
28	Quantum chemical topology and natural bond orbital analysis of Mâ€“O covalency in M(OC₆H₅)₄ (M = Ti, Zr, Hf, Ce, Th, Pa, U, Np). Physical Chemistry Chemical Physics, 2020, 22, 16804-16812.	1.3	29
29	Computational study of HCl adsorption on stoichiometric and oxygen vacancy PuO2 {111}, {110} and {100} surfaces. Journal of Nuclear Materials, 2020, 530, 151951.	1.3	11
30	Synthesis of a â€œMaskedâ€•Terminal Zinc Sulfide and Its Reactivity with BrÃ¸nsted and Lewis Acids. Angewandte Chemie, 2020, 132, 9032-9036.	1.6	1
31	Back-bonding between an electron-poor, high-oxidation-state metal and poor Ï€-acceptor ligand in a uranium(v)â€“dinitrogen complex. Nature Chemistry, 2019, 11, 806-811.	6.6	47
32	Computational analysis of Mâ€“O covalency in M(OC₆H₅)₄ (M = Ti,) Tj ETQq0 0 0 rgBT /Overloc	1.6	26
33	A manganese hydride molecular sieve for practical hydrogen storage under ambient conditions. Energy and Environmental Science, 2019, 12, 1580-1591.	15.6	41
34	Computational Study of the Bulk and Surface Properties of Minor Actinide Dioxides MAnO₂ (MAn = Np, Am, and Cm); Water Adsorption on Stoichiometric and Reduced {111}, {110}, and {100} Surfaces. Journal of Physical Chemistry C, 2019, 123, 15540-15550.	1.5	14
35	Computational study of H2 binding to MH3 (M = Ti, V, or Cr). Dalton Transactions, 2019, 48, 4921-4930.	1.6	2
36	High Uptake of ReO₄^{â”} and CO₂ Conversion by a Radiationâ€Resistant Thoriumâ€“Nickle [Th₄₈Ni₆] Nanocageâ€Based Metalâ€“Organic Framework. Angewandte Chemie - International Edition, 2019, 58, 6022-6027.	7.2	109

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37	Interactions of HCl and H2O with the surface of PuO2. Journal of Nuclear Materials, 2019, 518, 256-264.	1.3	8
38	Emergence of the structure-directing role of f-orbital overlap-driven covalency. Nature Communications, 2019, 10, 634.	5.8	50
39	Surface speciation and interactions between adsorbed chloride and water on cerium dioxide. Journal of Solid State Chemistry, 2018, 262, 16-25.	1.4	5
40	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.	1.5	45
41	High Spin Ground States in Matryoshka Actinide Nanoclusters: Aâ€‰Computational Study. Chemistry - A European Journal, 2018, 24, 347-350.	1.7	5
42	Frontispiece: Transuranic Computational Chemistry. Chemistry - A European Journal, 2018, 24, .	1.7	0
43	Uncovering the Origin of Divergence in the CsM(CrO₄)₂ (M = La, Pr, Nd, Sm,) Tj ETQq1 1 0.784314 rgBT /Ove Structure Analysis. Journal of the American Chemical Society, 2018, 140, 1674-1685.	6.6	14
44	Transuranic Computational Chemistry. Chemistry - A European Journal, 2018, 24, 2815-2825.	1.7	47
45	The performance of density functional theory for the description of ground and excited state properties of inorganic and organometallic uranium compounds. Journal of Organometallic Chemistry, 2018, 857, 58-74.	0.8	30
46	Energy-Degeneracy-Driven Covalency in Actinide Bonding. Journal of the American Chemical Society, 2018, 140, 17977-17984.	6.6	108
47	Post Hartreeâ€“Fock calculations of pnictogenâ€“uranium bonding in EUF₃ (E = Nâ€“Bi). Chemical Communications, 2018, 54, 11100-11103.	2.2	6
48	Characterisation and heat treatment of chloride-contaminated and humidified PuO2 samples. Journal of Nuclear Materials, 2018, 509, 654-666.	1.3	10
49	Multiple water layers on AnO2 {111}, {110}, and {100} surfaces (An = U, Pu): A computational study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	0.9	9
50	The shortest Thâ€“Th distance from a new type of quadruple bond. Physical Chemistry Chemical Physics, 2017, 19, 5070-5076.	1.3	28
51	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.	1.5	48
52	Seventeenâ€Coordinate Actinide Helium Complexes. Angewandte Chemie, 2017, 129, 7172-7175.	1.6	2
53	Seventeenâ€Coordinate Actinide Helium Complexes. Angewandte Chemie - International Edition, 2017, 56, 7066-7069.	7.2	12
54	Computational study of Anâ€“X bonding (An = Th, U; X = p-block-based ligands) in pyrrolic macrocycle-supported complexes from the quantum theory of atoms in molecules and bond energy decomposition analysis. Dalton Transactions, 2017, 46, 760-769.	1.6	12

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55	Thorium(IV) and Uranium(IV) trans-Calix[2]benzene[2]pyrrolide Alkyl and Alkynyl Complexes: Synthesis, Reactivity, and Electronic Structure. Organometallics, 2017, 36, 4669-4681.	1.1	24
56	Synthesis and Redox Chemistry of a Tantalum Alkylidene Complex Bearing a Metallaimidazole Ring. Organometallics, 2017, 36, 3520-3529.	1.1	7
57	Ionic adsorption on the brucite (0001) surface: A periodic electrostatic embedded cluster method study. Journal of Chemical Physics, 2016, 145, 204708.	1.2	7
58	Organometallic neptunium(III) complexes. Nature Chemistry, 2016, 8, 797-802.	6.6	88
59	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.	1.3	30
60	Uranium Metallaâ€Allenes with Carbene Imido R₂C=U^{IV}=NRâ€² Units (R=Ph₂PNSiMe₃; Râ€²=CPh₃): Alkaliâ€Metalâ€Mediated Pushâ€“Pull Effects with an Amido Auxiliary. Chemistry - A European Journal, 2016, 22, 11554-11558.	1.7	33
61	Catalyst: Nuclear Power in the 21 st Century. CheM, 2016, 1, 659-662.	5.8	36
62	Formation of a Ce(IV) Oxo Complex via Inner Sphere Nitrate Reduction. Journal of the American Chemical Society, 2016, 138, 12743-12746.	6.6	63
63	Uraniumâ€“Carbeneâ€“Imido Metallaâ€Allenes: Ancillaryâ€Ligandâ€Controlled cisâ€/transâ€Isomerisation and Assessment of trans Influence in the R₂C=U^{IV}=NRâ€² Unit (R=Ph₂PNSiMe₃;) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.7	37
64	Identification of a new electron-transfer relaxation pathway in photoexcited pyrrole dimers. Nature Communications, 2016, 7, 11357.	5.8	15
65	Covalency hinders AnO₂(H₂O)⁺ â†' AnO(OH)₂⁺ isomerisation (An = Paâ€“Pu). Dalton Transactions, 2016, 45, 3158-3162.	1.6	44
66	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.	1.0	14
67	Metalâ€“Metal Bonding in Uraniumâ€“Group 10 Complexes. Journal of the American Chemical Society, 2016, 138, 3333-3345.	6.6	79
68	The importance of second shell effects in the simulation of hydrated Sr2+ hydroxide complexes. Dalton Transactions, 2015, 44, 11572-11581.	1.6	9
69	The strength of actinideâ€“element bonds from the quantum theory of atoms-in-molecules. Dalton Transactions, 2015, 44, 2554-2566.	1.6	72
70	Electron localization in a mixed-valence diniobium benzene complex. Chemical Science, 2015, 6, 993-1003.	3.7	22
71	Synthesis, molecular and electronic structure, and reactions of a Znâ€“Hgâ€“Zn bonded complex. Chemical Communications, 2015, 51, 5743-5746.	2.2	13
72	Characterizing Pressureâ€Induced Uranium Cï£¿H Agostic Bonds. Angewandte Chemie - International Edition, 2015, 54, 6735-6739.	7.2	52

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73	Thoriumâ€“ligand multiple bonds via reductive deprotection of a trityl group. Chemical Science, 2015, 6, 3891-3899.	3.7	55
74	Probing the Limits of Alkaline Earthâ€“Transition Metal Bonding: An Experimental and Computational Study. Journal of the American Chemical Society, 2015, 137, 12352-12368.	6.6	30
75	Variable photon energy photoelectron spectroscopy of tris-cyclopentadienyl lanthanides. Dalton Transactions, 2014, 43, 5134-5141.	1.6	8
76	Stable GaX2, InX2 and TlX2 radicals. Nature Chemistry, 2014, 6, 315-319.	6.6	101
77	Switchable Ï€-coordination and Câ€“H metallation in small-cavity macrocyclic uranium and thorium complexes. Chemical Science, 2014, 5, 756-765.	3.7	53
78	Reductive silylation of a uranyl dibenzoylmethanate complex: an example of controlled uranyl oxo ligand cleavage. Chemical Science, 2014, 5, 3204-3213.	3.7	34
79	Synthesis and Spectroscopic and Computational Characterization of the Chalcogenido-Substituted Analogues of the Uranyl Ion, [OUE]²⁺ (E = S, Se). Journal of the American Chemical Society, 2013, 135, 5352-5355.	6.6	81
80	Systematic Investigation of Thorium(IV)â€“ and Uranium(IV)â€“Ligand Bonding in Dithiophosphonate, Thioselenophosphinate, and Diselenophosphonate Complexes. Inorganic Chemistry, 2013, 52, 10623-10631.	1.9	49
81	Do QTAIM metrics correlate with the strength of heavy elementâ€“ligand bonds?. Dalton Transactions, 2013, 42, 13477.	1.6	80
82	Synthesis and reactions of Î²-diketiminate-supported complexes with Mgâ€“Fe or Ybâ€“Fe bonds. Chemical Communications, 2013, 49, 3315.	2.2	49
83	A Generic Oneâ€Pot Route to Acyclic Twoâ€Coordinate Silylenes from Silicon(IV) Precursors: Synthesis and Structural Characterization of a Silylsilylene. Angewandte Chemie - International Edition, 2013, 52, 568-571.	7.2	138
84	Does Covalency Increase or Decrease across the Actinide Series? Implications for Minor Actinide Partitioning. Inorganic Chemistry, 2013, 52, 3407-3413.	1.9	285
85	Uncovering f-element bonding differences and electronic structure in a series of 1â€‰:â€‰3 and 1â€‰:â€‰4 complexes with a diselenophosphinate ligand. Chemical Science, 2013, 4, 1189.	3.7	146
86	A computational comparison of the speciation of uranyl D-gluconate and uranyl Î±-isosaccharinate complexes in aqueous solutions.. Materials Research Society Symposia Proceedings, 2012, 1475, 599.	0.1	0
87	Towards Hydrazine Based Hydrogen Storage Materials Incorporating Late Transition Metals: a DFT Study. Energy Procedia, 2012, 29, 585-593.	1.8	2
88	Inter- and intramolecular reactions of 1-deoxy-1-thio-1,6-anhydrosugars with Î±-diazoesters: synthesis of the tagetitoxin core by photochemical ylide rearrangement. Organic and Biomolecular Chemistry, 2012, 10, 8616.	1.5	11
89	Is gluconate a good model for isosaccharinate in uranyl(vi) chemistry? A DFT study. Dalton Transactions, 2012, 41, 5542.	1.6	9
90	Are Metalâ€“Metal Interactions Involved in the Rising Enthalpies Observed in The Kubas Binding of H₂ to Hydrazine-Linked Hydrogen Storage Materials?. Journal of Physical Chemistry C, 2012, 116, 19134-19144.	1.5	20

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91	Synthesis, Molecular and Electronic Structure of U^V(O)[N(SiMe₃)₂]₃. Inorganic Chemistry, 2012, 51, 1625-1633.	1.9	109
92	A Stable Two-Coordinate Acyclic Silylene. Journal of the American Chemical Society, 2012, 134, 6500-6503.	6.6	387
93	Bonding Trends Traversing the Tetravalent Actinide Series: Synthesis, Structural, and Computational Analysis of An^{IV}(^{Ar}acnac)₄ Complexes (An = Th, U, Np, Pu;) Tj ETQq1 1 0.784314 rgBT /Overlock 8557-8566.	1.9	76
94	The first group 4 metal bis(imido) and tris(imido) complexes. Chemical Science, 2012, 3, 819-824.	3.7	37
95	The Kubas interaction in M(ii) (M = Ti, V, Cr) hydrazine-based hydrogen storage materials: a DFT study. Dalton Transactions, 2012, 41, 8515.	1.6	50
96	Transition Metal Hydrazideâ€Based Hydrogenâ€Storage Materials: the First Atomsâ€Inâ€Molecules Analysis of the Kubas Interaction. Chemistry - A European Journal, 2012, 18, 1750-1760.	1.7	25
97	The coordination of Sr2+ by hydroxide: a density functional theoretical study. Dalton Transactions, 2011, 40, 11258.	1.6	8
98	Computational investigation of the speciation of uranyl gluconate complexes in aqueous solution. Dalton Transactions, 2011, 40, 11248.	1.6	12
99	Does covalency really increase across the 5f series? A comparison of molecular orbital, natural population, spin and electron density analyses of AnCp₃(An = Thâ€“Cm; Cp =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	1.6	150
100	Probing the Reactivity and Electronic Structure of a Uranium(V) Terminal Oxo Complex. Journal of the American Chemical Society, 2011, 133, 14224-14227.	6.6	96
101	Heterobimetallic Complexes Containing Caâ€“Fe or Ybâ€“Fe Bonds: Synthesis and Molecular and Electronic Structures of [M{CpFe(CO)₂}₂(THF)₃]₂(M) Tj ETQq1 1 0.784314 rgBT	6.6	38
102	Small Molecule Activation by Uranium Tris(aryloxides): Experimental and Computational Studies of Binding of N₂, Coupling of CO, and Deoxygenation Insertion of CO₂under Ambient Conditions. Journal of the American Chemical Society, 2011, 133, 9036-9051.	6.6	218
103	Group 3 and Lanthanide Boryl Compounds: Syntheses, Structures, and Bonding Analyses of Scâ”B, Yâ”B, and Luâ”B Ïƒ-Coordinated NHC Analogues. Journal of the American Chemical Society, 2011, 133, 3836-3839.	6.6	102
104	DFT studies of reductive elimination, Câ€“H activation and Î²-hydride elimination in alkyl and aryl palladium amine complexes. Theoretical Chemistry Accounts, 2011, 129, 303-312.	0.5	5
105	Quantum Chemical Studies of the Hydration of Sr²⁺ in Vacuum and Aqueous Solution. Chemistry - A European Journal, 2011, 17, 5060-5067.	1.7	17
106	All-electron CASPT2 study of Ce(Î·8â€“C8H6)2. Comptes Rendus Chimie, 2010, 13, 853-859.	0.2	23
107	Covalency in Ce^{IV} and U^{IV} Halide and Nâ€Heterocyclic Carbene Bonds. Chemistry - A European Journal, 2010, 16, 9623-9629.	1.7	137
108	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2010, , 1893-2012.		8

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109	Computational Study of Silica-Supported Transition Metal Fragments for Kubas-type Hydrogen Storage. Journal of the American Chemical Society, 2010, 132, 17296-17305.	6.6	30
110	The Reaction Chemistry of Plutonyl(VI) Chloride Complexes with Triphenyl Phosphineoxide and Triphenyl Phosphinimine. Inorganic Chemistry, 2010, 49, 9554-9562.	1.9	27
111	Covalency in AnCp4 (An = Thâ€“Cm): a comparison of molecular orbital, natural population and atoms-in-molecules analyses. Dalton Transactions, 2010, 39, 6719.	1.6	153
112	Variable Photon Energy Photoelectron Spectroscopy and Magnetism of YbCp₃ and LuCp₃. Organometallics, 2010, 29, 4752-4755.	1.1	13
113	Are the Ground States of the Later Actinocenes Multiconfigurational? All-Electron Spinâ^'Orbit Coupled CASPT2 Calculations on An(Î·⁸-C₈H₈)₂(An =) Tj ETQq1 1 0.784314 rgBT /C	1.1	31
114	Is Cerocene Really a Ce(III) Compound? All-Electron Spinâ^'Orbit Coupled CASPT2 Calculations on M(Î·⁸-C₈H₈)₂(M = Th, Pa, Ce). Journal of Physical Chemistry A, 2009, 113, 2896-2905.	1.1	72
115	Neptunium(vi) chain and neptunium(vi/v) mixed valence cluster complexes. Chemical Communications, 2009, , 917.	2.2	47
116	A mystery solved? Photoelectron spectroscopic and quantum chemical studies of the ion states of CeCp3+. Dalton Transactions, 2009, , 5943.	1.6	21
117	Theoretical Studies of the Electronic Structure of Compounds of the Actinide Elements. , 2008, , 1893-2012.		31
118	Tetravalent Metal Complexation by Keggin and Lacunary Phosphomolybdate Anions. Inorganic Chemistry, 2008, 47, 5787-5798.	1.9	39
119	Quantum chemical calculations on a selection of iodine-containing species (IO, OIO, INO3, (IO)2, I2O3,) Tj ETQq1 1 0.784314 rgBT /Ove	1.3	79
120	Covalency in the f Elementâ^'Chalcogen Bond. Computational Studies of M[N(EPR₂)₂]₃ (M = La, Ce, Pr, Pm, Eu, U, Np, Pu, Am, Cm; E = O, S, Se,) Tj ETQq0 0 0 rgBT /Overl	1.9	108
121	Experimental and Theoretical Comparison of Actinide and Lanthanide Bonding in M[N(EPR₂)₂]₃ Complexes (M = U, Pu, La, Ce; E = S, Se, Te; R = Ph,) Tj ETQq1 1 0.784314 rgBT /O	1.9	178
122	Mono(arene) Complexes of Thallium(I) Supported by a Weakly Coordinating Anion. Organometallics, 2007, 26, 1811-1815.	1.1	34
123	Actinyl chemistry across the U, Np and Pu series. Journal of Alloys and Compounds, 2007, 444-445, 453-456.	2.8	4
124	Covalency in the f-elementâ€“chalcogen bond. Journal of Alloys and Compounds, 2007, 444-445, 369-375.	2.8	44
125	Energy Decomposition Analysis of Metalâ^'Metal Bonding in [M2X8]2- (X = Cl, Br) Complexes of 5f (U, Np,) Tj ETQq1 1 0.784314 rgBT /O	1.9	38
126	Thallium(I) Sandwich, Multidecker, and Ether Complexes Stabilized by Weakly-Coordinating Anions:Â A Spectroscopic, Structural, and Theoretical Investigation. Journal of the American Chemical Society, 2007, 129, 881-894.	6.6	60

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127	A Structural and Theoretical Investigation of Equatorial cis and trans Uranyl Phosphinimine and Uranyl Phosphine Oxide Complexes UO2Cl2(Cy3PNH)2and UO2Cl2(Cy3PO)2. Inorganic Chemistry, 2007, 46, 4868-4875.	1.9	30
128	Metalâ€“metal bonding in molecular actinide compounds: electronic structure of [M2X8]2â^'(M = U, Np,) Tj ETQq0 0 0 rgBT /Overlock 1 5476-5483.	1.6	39
129	An ab initio study of the electronic structure of BCl2+3 and its decomposition pathways. Physical Chemistry Chemical Physics, 2006, 8, 1271.	1.3	3
130	Density functional theory investigation of the geometric and electronic structures of [UO2(H2O)m(OH)n]2â^'n(n + m = 5). Dalton Transactions, 2006, , 2403-2414.	1.6	60
131	Zinc(II) Î·1- and Î·2-Toluene Complexes:Â Structure and Bonding in Zn(C6F5)2Â·(toluene) and Zn(C6F4-2-C6F5)2Â·(toluene). Organometallics, 2006, 25, 3311-3313.	1.1	43
132	Bond-Forming Reactions of Dications with Molecules:â€‰ A Computational and Experimental Study of the Mechanisms for the Formation of HCF2+ from CF32+ and H2. Journal of Physical Chemistry A, 2006, 110, 2898-2905.	1.1	36
133	Density Functional Theory-Based Prediction of Some Aqueous-Phase Chemistry of Superheavy Element 111. Roentgenium(I) Is the â€˜Softest' Metal Ion. Inorganic Chemistry, 2006, 45, 10780-10785.	1.9	23
134	Trivalent [(C5Me5)2(THF)Ln]2(Î¼-Î·2:Î·2-N2) Complexes as Reducing Agents Including the Reductive Homologation of CO to a Ketene Carboxylate, (Î¼-Î·4-O2CCCO)2-. Journal of the American Chemical Society, 2006, 128, 14176-14184.	6.6	113
135	On the Paucity of Molecular Actinide Complexes with Unsupported Metalâ^'Metal Bonds:Â A Comparative Investigation of the Electronic Structure and Metalâ^'Metal Bonding in U2X6(X = Cl, F, OH, NH2, CH3) Complexes and d-Block Analogues. Inorganic Chemistry, 2006, 45, 6828-6839.	1.9	50
136	Planar Trimethylenemethane Dianion Chemistry of Lanthanide Metallocenes:Â Synthesis, Structure, Density Functional Theory Analysis, and Reactivity of [(C5Me5)2Ln]2[Î¼-Î·3:Î·3-C(CH2)3] Complexes. Journal of the American Chemical Society, 2006, 128, 16178-16189.	6.6	21
137	Photoelectron spectroscopy of Ce(Î·-C5H5)3 â€“ Accessing two ion states on 4f ionization. Chemical Physics Letters, 2006, 432, 17-21.	1.2	16
138	Time dependent DFT study of the electronic transition energies of RuO4 and OsO4. Chemical Physics Letters, 2005, 415, 64-68.	1.2	21
139	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
140	Nature of the Transition Metalâ^'Cycloheptatrienyl Bond. Computational Studies of the Electronic Structure of [M(Î·7-C7H7)(Î·5-C5H5)] (M = groups 4â^'6). Organometallics, 2005, 24, 1189-1197.	1.1	51
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