Ulf Wahlgren

List of Publications by Year
in descending order

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82	4,584	94433 37	98798 67
papers	citations	h-index	g-index

85	85	85	2956
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Probing the Nature of Chemical Bonding in Uranyl(VI) Complexes with Quantum Chemical Methods. Journal of Physical Chemistry A, 2012, 116, 12373-12380.	2.5	113
2	Effects of the first hydration sphere and the bulk solvent on the spectra of the f2isoelectronic actinide compounds: U4+, NpO2+, and PuO22+. Physical Chemistry Chemical Physics, 2010, 12, 1116-1130.	2.8	26
3	Charge Transfer in Uranyl(VI) Halides [UO₂X₄]^{2â^'} (X = F, Cl, Br,) Tj ETQq1 1 0.784314 rgBT /Ov 3615-3621.	2.5	21
4	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f actinide species. Journal of Chemical Physics, 2009, 131, 054107.	3.0	49
5	On the combined use of discrete solvent models and continuum descriptions of solvent effects in ligand exchange reactions: a case study of the uranyl(VI) aquo ion. Theoretical Chemistry Accounts, 2009, 124, 377-384.	1.4	22
6	Water Exchange Mechanism in the First Excited State of Hydrated Uranyl(VI). Inorganic Chemistry, 2009, 48, 11310-11313.	4.0	14
7	An Investigation of the Accuracy of Different DFT Functionals on the Water Exchange Reaction in Hydrated Uranyl(VI) in the Ground State and the First Excited State. Journal of Chemical Theory and Computation, 2008, 4, 569-577.	5.3	64
8	Ab Initio Study of the Mechanism for Photoinduced Yl-Oxygen Exchange in Uranyl(VI) in Acidic Aqueous Solution. Journal of the American Chemical Society, 2008, 130, 11742-11751.	13.7	28
9	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: A comparison between wave-function theory and density functional theory. Journal of Chemical Physics, 2007, 127, 214302.	3.0	75
10	Comment on â€œThe Waterâ€Exchange Mechanism of the [UO₂(OH₂)₅]²⁺ Ion Revisited: The Importance of a Proper Treatment of Electron Correlationâ€•[F. P. Rotzinger Chem. Eur. J., 2007, 13, 800]. Chemistry - A European Journal, 2007, 13, 10294-10297.	3.3	11
11	A theoretical study of the fluoride exchange between UO2F+(aq) and UO22+(aq). Dalton Transactions, 2006, , 3638.	3.3	14
12	Quantum Chemical Calculations of Reduction Potentials of AnO22+/AnO2+ (An = U, Np, Pu, Am) and Fe3+/Fe2+ Couples. Journal of Physical Chemistry A, 2006, 110, 9175-9182.	2.5	71
13	Actinide Chemistry in Solution, Quantum Chemical Methods and Models. Theoretical Chemistry Accounts, 2006, 115, 145-160.	1.4	114
14	Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4950-4956.	2.5	11
15	Spinâ^'Orbit Effects in Electron Transfer in Neptunyl(VI)â^'Neptunyl(V) Complexes in Solution. Journal of Physical Chemistry A, 2005, 109, 4957-4960.	2.5	14
16	The Mechanism of Water Exchange in AmO2(H2O)52+ and in the Isoelectronic UO2(H2O)5+ and NpO2(H2O)52+ Complexes as Studied by Quantum Chemical Methods. Journal of the American Chemical Society, 2004, 126, 7766-7767.	13.7	63
17	Electron Transfer in Uranyl(VI)â^'Uranyl(V) Complexes in Solution. Journal of the American Chemical Society, 2004, 126, 9801-9808.	13.7	37
18	Ab Initio Studies of Np and Pu Complexes and Reactions in the Gas Phase:â€‰ Structures and Thermodynamics. Journal of Physical Chemistry A, 2003, 107, 9705-9711.	2.5	21

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19	The performance of density functional theory for LnF (Ln=Nd, Eu, Gd, Yb) and YbH. Theoretical Chemistry Accounts, 2003, 110, 118-125.	1.4	41
20	Structure and Bonding in Solution of Dioxouranium(VI) Oxalate Complexes:Â Isomers and Intramolecular Ligand Exchange. Inorganic Chemistry, 2003, 42, 1982-1993.	4.0	68
21	Reduction of Uranyl(VI) by Iron(II) in Solutions:â€‰ An Ab Initio Study. Journal of Physical Chemistry A, 2003, 107, 587-592.	2.5	24
22	Mechanisms of Ligand Exchange Reactions, A Quantum Chemical Study of the Reaction UO22+(Aq) + HF(Aq) â† UO2F+(Aq) + H+(Aq). Journal of Physical Chemistry A, 2003, 107, 9456-9462.	2.5	12
23	Chelate Effect and Thermodynamics of Metal Complex Formation in Solution:Â A Quantum Chemical Study. Journal of the American Chemical Society, 2003, 125, 14941-14950.	13.7	78
24	Rates and Mechanism of Fluoride and Water Exchange in UO2F53-and [UO2F4(H2O)]2-Studied by NMR Spectroscopy and Wave Function Based Methods. Inorganic Chemistry, 2002, 41, 5626-5633.	4.0	37
25	Structure and Thermodynamics of Uranium(VI) Complexes in the Gas Phase: A Comparison of Experimental and ab Initio Data. Journal of Physical Chemistry A, 2002, 106, 11277-11282.	2.5	49
26	The gas phase structures of tungsten chlorides: density functional theory calculations on WCl6, WCl5, WCl4, WCl3 and W2Cl6â€Šâ€. Dalton Transactions RSC, 2001, , 1616-1620.	2.3	15
27	Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry. Inorganic Chemistry, 2001, 40, 3516-3525.	4.0	138
28	The Mechanism for Water Exchange in [UO2(H2O)5]2+and [UO2(oxalate)2(H2O)]2-, as Studied by Quantum Chemical Methods. Journal of the American Chemical Society, 2001, 123, 11999-12008.	13.7	123
29	A theoretical study of the chemisorption of molecular hydrogen on a seven atom gold cluster. Journal of Molecular Structure, 2001, 567-568, 137-143.	3.6	13
30	Spinâ€“orbit coupling within a two-component density functional theory approach: theory, implementation and first applications. Chemical Physics Letters, 2001, 344, 207-212.	2.6	34
31	Rates and Mechanisms of Water Exchange of UO22+(aq) and UO2(oxalate)F(H2O)2-:Â A Variable-Temperature17O and19F NMR Study. Inorganic Chemistry, 2000, 39, 799-805.	4.0	102
32	Reduction of uranyl by hydrogen: an ab initio study. Chemical Physics, 1999, 244, 185-193.	1.9	81
33	Investigation of the low-lying excited states of PuO22+. Chemical Physics, 1999, 244, 195-201.	1.9	42
34	Reduction Behavior of the Early Actinyl Ions in Aqueous Solution. Journal of Physical Chemistry A, 1999, 103, 9285-9289.	2.5	54
35	On the efficiency of an effective Hamiltonian in spin-orbit CI calculations. Chemical Physics Letters, 1998, 286, 261-266.	2.6	47
36	On the combination of ECP-based CI calculations with all-electron spin-orbit mean-field integrals. Chemical Physics Letters, 1998, 286, 267-271.	2.6	64

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37	A local approximation for relativistic scalar operators applied to the uranyl ion and to Au2. Chemical Physics Letters, 1998, 287, 525-530.	2.6	35
38	Spin-orbit effects in the PtH+2 ion. Computational and Theoretical Chemistry, 1998, 451, 227-235.	1.5	8
39	Ab initio calculations of the ${} ^2{i P}_{{ 1}over { 2}} hbox{-}{} ^2{i P}_{{ 3} over { 2}} $ splitting in the thallium atom. Theoretical Chemistry Accounts, 1997, 97, 324-330.	1.4	30
40	DFT and MO calculations of atomic and molecular chemisorption energies on surface cluster models. Theoretica Chimica Acta, 1996, 94, 297-310.	0.8	19
41	Chemisorption of hydrogen and oxygen atoms on a cobalt surface: A quantum chemical cluster model study. International Journal of Quantum Chemistry, 1996, 57, 105-111.	2.0	9
42	A new mean-field and ECP-based spin-orbit method. Applications to Pt and PtH. Chemical Physics Letters, 1996, 251, 357-364.	2.6	131
43	A mean-field spin-orbit method applicable to correlated wavefunctions. Chemical Physics Letters, 1996, 251, 365-371.	2.6	1,008
44	Calculations of hydrogen chemisorption energies on optimized copper clusters. Chemical Physics Letters, 1995, 237, 550-559.	2.6	39
45	New relativistic effective core potentials for heavy elements. Chemical Physics, 1995, 201, 357-362.	1.9	35
46	On the accuracy of gradient corrected density functional methods for transition metal complexes. Journal of Chemical Physics, 1995, 102, 872-878.	3.0	74
47	Relativistic calculations on platinum hydride using effective core potentials and firstâ€order perturbation theory. Journal of Chemical Physics, 1992, 96, 8363-8366.	3.0	19
48	A theoretical study of atomic oxygen chemisorption on the Ni(100) and Ni(111) surfaces. International Journal of Quantum Chemistry, 1992, 42, 1149-1169.	2.0	46
49	The Effective Core Potential Method. Lecture Notes in Quantum Chemistry II, 1992, , 413-421.	0.3	3
50	A Cluster Model for Reactions on Transition Metal Surfaces. , 1992, , 37-65.		2
51	Chemisorption on Metal Surfaces. A Cluster Model Approach. Topics in Molecular Organization and Engineering, 1992, , 1-17.	0.1	0
52	Model Studies of Chemisorption on Platinum Surfaces. NATO ASI Series Series B: Physics, 1992, , 453-461.	0.2	0
53	A theoretical study of the chemisorption of methane on a Ni(100) surface. Chemical Physics, 1991, 156, 379-386.	1.9	49
54	Are atomic 3d-anisotropies important for chemisorption of hydrogen on cobalt?. Chemical Physics Letters, 1991, 177, 49-53.	2.6	2

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55	Oxygen chemisorption on metal surfaces using the cluster model: Basis set effects. Theoretica Chimica Acta, 1991, 79, 413-418.	0.8	4
56	Relativistic quantum calculations on some mercury sulfide molecules. Water, Air, and Soil Pollution, 1991, 56, 681-695.	2.4	33
57	A theoretical study of atomic fluorine chemisorption on the Ni(100) surface. Journal of Chemical Physics, 1991, 94, 4024-4030.	3.0	52
58	Theoretical calculations on the structure of the hexahydrated divalent zinc, cadmium and mercury ions. Chemical Physics Letters, 1990, 172, 49-54.	2.6	30
59	The effects of core (3d) correlation on chemisorption. Journal of Chemical Physics, 1990, 93, 4954-4957.	3.0	21
60	Mechanism for H2 Dissociation on Transition Metal Clusters and Surfaces. ACS Symposium Series, 1989, , 125-139.	0.5	1
61	Cu 3d covalency in chemisorption?. Journal of Chemical Physics, 1989, 90, 4613-4616.	3.0	35
62	The mechanism for the O2 dissociation on Ni(100). Journal of Chemical Physics, 1989, 90, 6791-6801.	3.0	50
63	Non-relativistic and relativistic calculations on some Zn, Cd and Hg complexes. Chemical Physics, 1989, 133, 207-219.	1.9	33
64	A comparison of the on-top dissociation of H2 on Ni(100) and Cu(100). Theoretica Chimica Acta, 1989, 75, 143-159.	0.8	36
65	On the cluster convergence of chemisorption energies. Chemical Physics Letters, 1988, 149, 265-272.	2.6	181
66	Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. Theoretica Chimica Acta, 1988, 74, 167-184.	0.8	66
67	Ab initio investigation of methyl adsorption on Ni(111). Computational and Theoretical Chemistry, 1988, 170, 151-153.	1.5	3
68	Bonding and electronic structure in diatomic ThO: Quasirelativistic effective core potential calculations. Computational and Theoretical Chemistry, 1988, 169, 339-354.	1.5	50
69	A theoretical study of methyl chemisorption on Ni(111). Journal of Chemical Physics, 1988, 89, 6982-6988.	3.0	92
70	Model studies of the chemisorption of hydrogen and oxygen on Cu(100). Physical Review B, 1987, 36, 7389-7401.	3.2	107
71	Effective core potential parameters for firstâ€•and secondâ€•row atoms. Journal of Chemical Physics, 1987, 86, 2176-2184.	3.0	109
72	Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. I. The design of a one-electron effective core potential which includes 3d relaxation effects. Chemical Physics, 1987, 112, 325-337.	1.9	86

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73	A theoretical study of the geometrical properties of tellurite complexes. Chemical Physics, 1985, 100, 229-235.	1.9	9
74	CAS SCF ECP calculations on the optical spectrum of Mo2(O2CH)4 and on the barrier to internal rotation in Mo2Cl84â^'. Chemical Physics Letters, 1985, 118, 389-394.	2.6	5
75	Effective core potential calculation using frozen orbitals applications on the fourth period main group elements. Journal of Chemical Physics, 1984, 80, 1593-1596.	3.0	19
76	CAS SCF calculations using effective core potentials on the optical spectrum of Mo2Cl84â^'. Chemical Physics Letters, 1984, 104, 336-342.	2.6	8
77	Effective core potential calculations using frozen orbitals. Applications to transition metals. Chemical Physics, 1983, 80, 7-16.	1.9	145
78	Investigations of heavily contracted basis sets and superposition errors for some first- and second-row transition elements. Chemical Physics Letters, 1982, 89, 26-30.	2.6	3
79	Valence photoelectron spectrum of CoO.Ab initio calculations of energies and relative intensities within a limitedCI framework. International Journal of Quantum Chemistry, 1979, 15, 403-410.	2.0	3
80	Pseudo-potential calculations on O, S, Ni, H2S and H2O. Applications of a comparatively simple parameter fitting scheme. Chemical Physics, 1978, 29, 231-240.	1.9	9
81	Ab-initio and pseudo-potential calculations on some first, second and third row molecules. A comparative study. Chemical Physics, 1978, 32, 215-221.	1.9	16
82	Hydrogen bond studies. Theoretica Chimica Acta, 1973, 28, 161-168.	0.8	75