

Ulf Wahlgren

List of Publications by Year in descending order

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82
papers

4,584
citations

94433

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98798

67
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85
all docs

85
docs citations

85
times ranked

2956
citing authors

#	ARTICLE	IF	CITATIONS
1	A mean-field spin-orbit method applicable to correlated wavefunctions. <i>Chemical Physics Letters</i> , 1996, 251, 365-371.	2.6	1,008
2	On the cluster convergence of chemisorption energies. <i>Chemical Physics Letters</i> , 1988, 149, 265-272.	2.6	181
3	Effective core potential calculations using frozen orbitals. Applications to transition metals. <i>Chemical Physics</i> , 1983, 80, 7-16.	1.9	145
4	Solvent Effects on Uranium(VI) Fluoride and Hydroxide Complexes Studied by EXAFS and Quantum Chemistry. <i>Inorganic Chemistry</i> , 2001, 40, 3516-3525.	4.0	138
5	A new mean-field and ECP-based spin-orbit method. Applications to Pt and PtH. <i>Chemical Physics Letters</i> , 1996, 251, 357-364.	2.6	131
6	The Mechanism for Water Exchange in $[\text{UO}_2(\text{H}_2\text{O})_5]^{2+}$ and $[\text{UO}_2(\text{oxalate})_2(\text{H}_2\text{O})]^{2-}$, as Studied by Quantum Chemical Methods. <i>Journal of the American Chemical Society</i> , 2001, 123, 11999-12008.	13.7	123
7	Actinide Chemistry in Solution, Quantum Chemical Methods and Models. <i>Theoretical Chemistry Accounts</i> , 2006, 115, 145-160.	1.4	114
8	Probing the Nature of Chemical Bonding in Uranyl(VI) Complexes with Quantum Chemical Methods. <i>Journal of Physical Chemistry A</i> , 2012, 116, 12373-12380.	2.5	113
9	Effective core potential parameters for first- and second-row atoms. <i>Journal of Chemical Physics</i> , 1987, 86, 2176-2184.	3.0	109
10	Model studies of the chemisorption of hydrogen and oxygen on Cu(100). <i>Physical Review B</i> , 1987, 36, 7389-7401.	3.2	107
11	Rates and Mechanisms of Water Exchange of $\text{UO}_2^{2+}(\text{aq})$ and $\text{UO}_2(\text{oxalate})(\text{H}_2\text{O})_2$: A Variable-Temperature ^{17}O and ^{19}F NMR Study. <i>Inorganic Chemistry</i> , 2000, 39, 799-805.	4.0	102
12	A theoretical study of methyl chemisorption on Ni(111). <i>Journal of Chemical Physics</i> , 1988, 89, 6982-6988.	3.0	92
13	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. <i>Chemical Physics</i> , 1987, 112, 325-337.	1.9	86
14	Reduction of uranyl by hydrogen: an ab initio study. <i>Chemical Physics</i> , 1999, 244, 185-193.	1.9	81
15	Chelate Effect and Thermodynamics of Metal Complex Formation in Solution: A Quantum Chemical Study. <i>Journal of the American Chemical Society</i> , 2003, 125, 14941-14950.	13.7	78
16	Hydrogen bond studies. <i>Theoretica Chimica Acta</i> , 1973, 28, 161-168.	0.8	75
17	Theoretical investigation of the energies and geometries of photoexcited uranyl(VI) ion: A comparison between wave-function theory and density functional theory. <i>Journal of Chemical Physics</i> , 2007, 127, 214302.	3.0	75
18	On the accuracy of gradient corrected density functional methods for transition metal complexes. <i>Journal of Chemical Physics</i> , 1995, 102, 872-878.	3.0	74

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19	Quantum Chemical Calculations of Reduction Potentials of AnO ₂₂₊ /AnO ₂₊ (An = U, Np, Pu, Am) and Fe ₃ /Fe ₂₊ Couples. <i>Journal of Physical Chemistry A</i> , 2006, 110, 9175-9182.	2.5	71
20	Structure and Bonding in Solution of Dioxouranium(VI) Oxalate Complexes: λ Isomers and Intramolecular Ligand Exchange. <i>Inorganic Chemistry</i> , 2003, 42, 1982-1993.	4.0	68
21	Model studies of the chemisorption of hydrogen and oxygen on nickel surfaces. <i>Theoretica Chimica Acta</i> , 1988, 74, 167-184.	0.8	66
22	On the combination of ECP-based CI calculations with all-electron spin-orbit mean-field integrals. <i>Chemical Physics Letters</i> , 1998, 286, 267-271.	2.6	64
23	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. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 569-577.	5.3	64
24	The Mechanism of Water Exchange in AmO ₂ (H ₂ O) ₅₂₊ and in the Isoelectronic UO ₂ (H ₂ O) ₅₊ and NpO ₂ (H ₂ O) ₅₂₊ Complexes as Studied by Quantum Chemical Methods. <i>Journal of the American Chemical Society</i> , 2004, 126, 7766-7767.	13.7	63
25	Reduction Behavior of the Early Actinyl Ions in Aqueous Solution. <i>Journal of Physical Chemistry A</i> , 1999, 103, 9285-9289.	2.5	54
26	A theoretical study of atomic fluorine chemisorption on the Ni(100) surface. <i>Journal of Chemical Physics</i> , 1991, 94, 4024-4030.	3.0	52
27	Bonding and electronic structure in diatomic ThO: Quasirelativistic effective core potential calculations. <i>Computational and Theoretical Chemistry</i> , 1988, 169, 339-354.	1.5	50
28	The mechanism for the O ₂ dissociation on Ni(100). <i>Journal of Chemical Physics</i> , 1989, 90, 6791-6801.	3.0	50
29	A theoretical study of the chemisorption of methane on a Ni(100) surface. <i>Chemical Physics</i> , 1991, 156, 379-386.	1.9	49
30	Structure and Thermodynamics of Uranium(VI) Complexes in the Gas Phase: A Comparison of Experimental and ab Initio Data. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11277-11282.	2.5	49
31	On the universality of the long-/short-range separation in multiconfigurational density-functional theory. II. Investigating f actinide species. <i>Journal of Chemical Physics</i> , 2009, 131, 054107.	3.0	49
32	On the efficiency of an effective Hamiltonian in spin-orbit CI calculations. <i>Chemical Physics Letters</i> , 1998, 286, 261-266.	2.6	47
33	A theoretical study of atomic oxygen chemisorption on the Ni(100) and Ni(111) surfaces. <i>International Journal of Quantum Chemistry</i> , 1992, 42, 1149-1169.	2.0	46
34	Investigation of the low-lying excited states of PuO ₂₂₊ . <i>Chemical Physics</i> , 1999, 244, 195-201.	1.9	42
35	The performance of density functional theory for LnF (Ln=Nd, Eu, Gd, Yb) and YbH. <i>Theoretical Chemistry Accounts</i> , 2003, 110, 118-125.	1.4	41
36	Calculations of hydrogen chemisorption energies on optimized copper clusters. <i>Chemical Physics Letters</i> , 1995, 237, 550-559.	2.6	39

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37	Rates and Mechanism of Fluoride and Water Exchange in UO ₂ F ₅ ³⁻ and [UO ₂ F ₄ (H ₂ O)] ²⁻ Studied by NMR Spectroscopy and Wave Function Based Methods. <i>Inorganic Chemistry</i> , 2002, 41, 5626-5633.	4.0	37
38	Electron Transfer in Uranyl(VI)~Uranyl(V) Complexes in Solution. <i>Journal of the American Chemical Society</i> , 2004, 126, 9801-9808.	13.7	37
39	A comparison of the on-top dissociation of H ₂ on Ni(100) and Cu(100). <i>Theoretica Chimica Acta</i> , 1989, 75, 143-159.	0.8	36
40	Cu 3d covalency in chemisorption?. <i>Journal of Chemical Physics</i> , 1989, 90, 4613-4616.	3.0	35
41	New relativistic effective core potentials for heavy elements. <i>Chemical Physics</i> , 1995, 201, 357-362.	1.9	35
42	A local approximation for relativistic scalar operators applied to the uranyl ion and to Au ₂ . <i>Chemical Physics Letters</i> , 1998, 287, 525-530.	2.6	35
43	Spin-orbit coupling within a two-component density functional theory approach: theory, implementation and first applications. <i>Chemical Physics Letters</i> , 2001, 344, 207-212.	2.6	34
44	Non-relativistic and relativistic calculations on some Zn, Cd and Hg complexes. <i>Chemical Physics</i> , 1989, 133, 207-219.	1.9	33
45	Relativistic quantum calculations on some mercury sulfide molecules. <i>Water, Air, and Soil Pollution</i> , 1991, 56, 681-695.	2.4	33
46	Theoretical calculations on the structure of the hexahydrated divalent zinc, cadmium and mercury ions. <i>Chemical Physics Letters</i> , 1990, 172, 49-54.	2.6	30
47	Ab initio calculations of the $\frac{1}{2} P_{1/2} - \frac{1}{2} P_{3/2}$ splitting in the thallium atom. <i>Theoretical Chemistry Accounts</i> , 1997, 97, 324-330.	1.4	30
48	Ab Initio Study of the Mechanism for Photoinduced Yl-Oxygen Exchange in Uranyl(VI) in Acidic Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2008, 130, 11742-11751.	13.7	28
49	Effects of the first hydration sphere and the bulk solvent on the spectra of the f ₂ isoelectronic actinide compounds: U ⁴⁺ , NpO ₂ ⁺ , and PuO ₂ ²⁺ . <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 1116-1130.	2.8	26
50	Reduction of Uranyl(VI) by Iron(II) in Solutions: An Ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 587-592.	2.5	24
51	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. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 377-384.	1.4	22
52	The effects of core (3d) correlation on chemisorption. <i>Journal of Chemical Physics</i> , 1990, 93, 4954-4957.	3.0	21
53	Ab Initio Studies of Np and Pu Complexes and Reactions in the Gas Phase: Structures and Thermodynamics. <i>Journal of Physical Chemistry A</i> , 2003, 107, 9705-9711.	2.5	21
54	Charge Transfer in Uranyl(VI) Halides [UO ₂ X ₄] ²⁻ (X = F, Cl, Br). <i>Journal of Physical Chemistry A</i> , 2003, 107, 3615-3621.	2.5	21

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55	Effective core potential calculation using frozen orbitals applications on the fourth period main group elements. <i>Journal of Chemical Physics</i> , 1984, 80, 1593-1596.	3.0	19
56	Relativistic calculations on platinum hydride using effective core potentials and first-order perturbation theory. <i>Journal of Chemical Physics</i> , 1992, 96, 8363-8366.	3.0	19
57	DFT and MO calculations of atomic and molecular chemisorption energies on surface cluster models. <i>Theoretica Chimica Acta</i> , 1996, 94, 297-310.	0.8	19
58	Ab-initio and pseudo-potential calculations on some first, second and third row molecules. A comparative study. <i>Chemical Physics</i> , 1978, 32, 215-221.	1.9	16
59	The gas phase structures of tungsten chlorides: density functional theory calculations on WCl ₆ , WCl ₅ , WCl ₄ , WCl ₃ and W ₂ Cl ₆ . <i>Dalton Transactions RSC</i> , 2001, , 1616-1620.	2.3	15
60	Spin-Orbit Effects in Electron Transfer in Neptunyl(VI)~Neptunyl(V) Complexes in Solution. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4957-4960.	2.5	14
61	A theoretical study of the fluoride exchange between UO ₂ F ⁺ (aq) and UO ₂ ²⁺ (aq). <i>Dalton Transactions</i> , 2006, , 3638.	3.3	14
62	Water Exchange Mechanism in the First Excited State of Hydrated Uranyl(VI). <i>Inorganic Chemistry</i> , 2009, 48, 11310-11313.	4.0	14
63	A theoretical study of the chemisorption of molecular hydrogen on a seven atom gold cluster. <i>Journal of Molecular Structure</i> , 2001, 567-568, 137-143.	3.6	13
64	Mechanisms of Ligand Exchange Reactions, A Quantum Chemical Study of the Reaction UO ₂ ²⁺ (Aq) + HF(Aq) → UO ₂ F ⁺ (Aq) + H ⁺ (Aq). <i>Journal of Physical Chemistry A</i> , 2003, 107, 9456-9462.	2.5	12
65	Electron Transfer in Neptunyl(VI)~Neptunyl(V) Complexes in Solution. <i>Journal of Physical Chemistry A</i> , 2005, 109, 4950-4956.	2.5	11
66	Comment on "The Water-Exchange Mechanism of the [UO ₂ (OH) ₂] ₅ ²⁺ Ion Revisited: The Importance of a Proper Treatment of Electron Correlation" [F. P. Rotzinger <i>Chem. Eur. J.</i>, 2007, <i>13</i>, 800]. <i>Chemistry - A European Journal</i> , 2007, 13, 10294-10297.	3.3	11
67	Pseudo-potential calculations on O, S, Ni, H ₂ S and H ₂ O. Applications of a comparatively simple parameter fitting scheme. <i>Chemical Physics</i> , 1978, 29, 231-240.	1.9	9
68	A theoretical study of the geometrical properties of tellurite complexes. <i>Chemical Physics</i> , 1985, 100, 229-235.	1.9	9
69	Chemisorption of hydrogen and oxygen atoms on a cobalt surface: A quantum chemical cluster model study. <i>International Journal of Quantum Chemistry</i> , 1996, 57, 105-111.	2.0	9
70	CAS SCF calculations using effective core potentials on the optical spectrum of Mo ₂ Cl ₈ ⁴⁻ . <i>Chemical Physics Letters</i> , 1984, 104, 336-342.	2.6	8
71	Spin-orbit effects in the PtH ₂ ion. <i>Computational and Theoretical Chemistry</i> , 1998, 451, 227-235.	1.5	8
72	CAS SCF ECP calculations on the optical spectrum of Mo ₂ (O ₂ CH) ₄ and on the barrier to internal rotation in Mo ₂ Cl ₈ ⁴⁻ . <i>Chemical Physics Letters</i> , 1985, 118, 389-394.	2.6	5

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73	Oxygen chemisorption on metal surfaces using the cluster model: Basis set effects. <i>Theoretica Chimica Acta</i> , 1991, 79, 413-418.	0.8	4
74	Valence photoelectron spectrum of CoO. Ab initio calculations of energies and relative intensities within a limited CI framework. <i>International Journal of Quantum Chemistry</i> , 1979, 15, 403-410.	2.0	3
75	Investigations of heavily contracted basis sets and superposition errors for some first- and second-row transition elements. <i>Chemical Physics Letters</i> , 1982, 89, 26-30.	2.6	3
76	Ab initio investigation of methyl adsorption on Ni(111). <i>Computational and Theoretical Chemistry</i> , 1988, 170, 151-153.	1.5	3
77	The Effective Core Potential Method. <i>Lecture Notes in Quantum Chemistry II</i> , 1992, , 413-421.	0.3	3
78	Are atomic 3d-anisotropies important for chemisorption of hydrogen on cobalt?. <i>Chemical Physics Letters</i> , 1991, 177, 49-53.	2.6	2
79	A Cluster Model for Reactions on Transition Metal Surfaces. , 1992, , 37-65.		2
80	Mechanism for H ₂ Dissociation on Transition Metal Clusters and Surfaces. <i>ACS Symposium Series</i> , 1989, , 125-139.	0.5	1
81	Chemisorption on Metal Surfaces. A Cluster Model Approach. <i>Topics in Molecular Organization and Engineering</i> , 1992, , 1-17.	0.1	0
82	Model Studies of Chemisorption on Platinum Surfaces. <i>NATO ASI Series Series B: Physics</i> , 1992, , 453-461.	0.2	0