Knut J BÃ¸rve

List of Publications by Year
in descending order

103 papers	2,215 citations	201674 27 h-index	276875 41 g-index
103 all docs	103 docs citations	103 times ranked	1831 citing authors

#	Article	IF	Citations
1	Activity of Rhodium-Catalyzed Hydroformylation:Â Added Insight and Predictions from Theory. Journal of the American Chemical Society, 2007, 129, 8487-8499.	13.7	94
2	Theoretical Models of Ethylene Polymerization over a Mononuclear Chromium(II)/Silica Site. Journal of Catalysis, 2000, 195, 125-139.	6.2	81
3	Carbon 1s photoelectron spectroscopy of CF4 and CO: Search for chemical effects on the carbon 1s hole-state lifetime. Journal of Chemical Physics, 2002, 116, 10221-10228.	3.0	80
4	Chemical Insights from High-Resolution X-ray Photoelectron Spectroscopy and ab Initio Theory:â€‰ Propyne, Trifluoropropyne, and Ethynylsulfur Pentafluoride. Journal of the American Chemical Society, 2001, 123, 10729-10737.	13.7	75
5	Molecular-Level Insight into Cr/Silica Phillips-Type Catalysts: Polymerization-Active Dinuclear Chromium Sites. Journal of Catalysis, 2002, 206, 331-338.	6.2	70
6	Activity of Homogeneous Chromium(III)-Based Alkene Polymerization Catalysts:Â Lack of Importance of the Barrier to Ethylene Insertion. Organometallics, 2000, 19, 403-410.	2.3	66
7	Molecular-Level Insight into Cr/Silica Phillips-Type Catalysts: Polymerization-Active Mononuclear Chromium Sites. Journal of Catalysis, 2002, 205, 366-374.	6.2	64
8	On the Origins of Coreâ^'Electron Chemical Shifts of Small Biomolecules in Aqueous Solution: Insights from Photoemission and ab Initio Calculations of Glycine_{aq}. Journal of the American Chemical Society, 2011, 133, 3120-3130.	13.7	61
9	An investigation of the quantum chemical description of the ethylenic double bond in reactions: II. Insertion of ethylene into a titanium-carbon bond. Journal of Computational Chemistry, 1998, 19, 947-960.	3.3	56
10	Nonstoichiometric Intensities in Core Photoelectron Spectroscopy. Physical Review Letters, 2012, 108, 193005.	7.8	51
11	High resolution photoelectron spectroscopy of sulfur 2p electrons in H2S, SO2, CS2, and OCS. Journal of Chemical Physics, 1996, 105, 9035-9039.	3.0	48
12	Ziegler-Natta Ethylene Insertion Reaction for a Five-Coordinate Titanium Chloride Complex Bridged to an Aluminum Hydride Cocatalyst. Journal of the American Chemical Society, 1995, 117, 4109-4117.	13.7	47
13	Fluorine as a Ï€ Donor. Carbon 1s Photoelectron Spectroscopy and Proton Affinities of Fluorobenzenes. Journal of Organic Chemistry, 2006, 71, 1961-1968.	3.2	47
14	Accurate and approximate calculations of Franckâ€“Condon intensities in the carbon 1s photoelectron spectrum of methane. Journal of Chemical Physics, 2000, 112, 7979-7985.	3.0	46
15	Catalytic dehydrogenation of ethane over mononuclear Cr(III) surface sites on silica. part I. Câ€”H activation by ĺƒâ€bond metathesis. Journal of Physical Organic Chemistry, 2004, 17, 990-1006.	1.9	44
16	Toward the Spectrum of Free Polyethylene:â€‰ Linear Alkanes Studied by Carbon 1s Photoelectron Spectroscopy and Theory. Journal of the American Chemical Society, 2002, 124, 7866-7873.	13.7	41
17	The Substituent Effect of the Methyl Group. Carbon 1s Ionization Energies, Proton Affinities, and Reactivities of the Methylbenzenes. Journal of Organic Chemistry, 2007, 72, 5715-5723.	3.2	40
18	Methane dissociation on a nonplanar MgO(001) surface. Theoretical modeling of surface defects. Journal of Chemical Physics, 1991, 95, 4626-4631.	3.0	39

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19	The ESCA moleculeâ€"Historical remarks and new results. Journal of Electron Spectroscopy and Related Phenomena, 2012, 185, 191-197.	1.7	37
20	Conformational Effects in Inner-Shell Photoelectron Spectroscopy of Ethanol. Physical Review Letters, 2005, 95, 103002.	7.8	35
21	Vibrational Structure and Vibronic Coupling in the Carbon 1s Photoelectron Spectra of Ethane and Deuteroethane. Journal of Physical Chemistry A, 2001, 105, 7700-7706.	2.5	34
22	Vibrational structure and vibronic coupling in the carbon 1s photoelectron spectra of benzene and deuterobenzene. Physical Chemistry Chemical Physics, 2002, 4, 5937-5943.	2.8	34
23	Size of neutral argon clusters from core-level photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2006, 8, 1891-1898.	2.8	34
24	Theoretical Analysis of dâ€"d Transitions for the Reduced Cr/Silica System. Catalysis Letters, 2001, 75, 49-54.	2.6	32
25	Theoretical Analysis of CO Adsorption on the Reduced Cr/Silica System. Journal of Catalysis, 2002, 205, 177-190.	6.2	32
26	Accuracy of Calculated Chemical Shifts in Carbon 1s Ionization Energies from Single-Reference ab Initio Methods and Density Functional Theory. Journal of Chemical Theory and Computation, 2011, 7, 4104-4114.	5.3	29
27	Carbon 1s photoelectron spectroscopy of six-membered cyclic hydrocarbons. Physical Chemistry Chemical Physics, 2004, 6, 4254-4259.	2.8	28
28	The local structure of small water clusters: imprints on the core-level photoelectron spectrum. Journal of Physics B: Atomic, Molecular and Optical Physics, 2009, 42, 055201.	1.5	27
29	On the calculation of molecular field splitting in S 2p photoelectron spectra. Chemical Physics Letters, 1996, 262, 801-806.	2.6	26
30	Quantum Chemical Investigation of Ethylene Insertion into the Crâ"CH3Bond in CrCl(H2O)CH3+as a Model of Homogeneous Ethylene Polymerization. Organometallics, 1997, 16, 2514-2522.	2.3	25
31	Evaluation of PM3(tm) as a Geometry Generator in Theoretical Studies of Transition-Metal-Based Catalysts for Polymerizing Olefins. Journal of Molecular Modeling, 1997, 3, 193-202.	1.8	25
32	Theoretical Investigation of Bis(imido)chromium(VI) Cations as Polymerization Catalysts. Organometallics, 2001, 20, 616-626.	2.3	24
33	Evidence of Fermi resonance in core-ionized methane. Journal of Chemical Physics, 2000, 112, 7986-7991.	3.0	23
34	Reactivity and Core-Ionization Energies in Conjugated Dienes. Carbon 1s Photoelectron Spectroscopy of 1,3-Pentadiene. Journal of Physical Chemistry A, 2005, 109, 5085-5092.	2.5	23
35	Lineshapes in carbon 1s photoelectron spectra of methanol clusters. Physical Chemistry Chemical Physics, 2006, 8, 2473-2482.	2.8	23
36	Additivity of Substituent Effects. Core-Ionization Energies and Substituent Effects in Fluoromethylbenzenes. Journal of Physical Chemistry A, 2009, 113, 3481-3490.	2.5	23

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37	Molecular adsorption of methane and methyl onto MgO(100) An embedded-cluster study. Surface Science, 1999, 421, 296-307.	1.9	22
38	Effects of molecular conformation on inner-shell ionization energies. Physical Chemistry Chemical Physics, 2007, 9, 719-724.	2.8	22
39	Structure and Thermodynamics of Gaseous Oxides, Hydroxides, and Mixed Oxohydroxides of Chromium:Â CrOm(OH)n(m,n= 0â‰¥2) and CrO3. A Computational Study. Journal of Physical Chemistry A, 1998, 102, 10414-10423.	2.5	21
40	Carbon 1s Photoelectron Spectroscopy of Halomethanes. Effects of Electronegativity, Hardness, Charge Distribution, and Relaxation. Journal of Physical Chemistry A, 2004, 108, 4983-4990.	2.5	21
41	Chemical shifts of carbon 1s ionization energies. Journal of Electron Spectroscopy and Related Phenomena, 2011, 183, 2-9.	1.7	21
42	Catalytic dehydrogenation of ethane over mononuclear Cr(III)-silica surface sites. Part 2: Cï£¿H activation by oxidative addition. Journal of Physical Organic Chemistry, 2006, 19, 25-33.	1.9	20
43	The O 1s photoelectron spectrum of molecular oxygen revisited. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 095101.	1.5	20
44	Molecular adsorption of NH3 on MgO(001) and hydrogen abstraction from NH3 on gaseous LiO and Liâ€doped MgO(001). A computational study. Journal of Chemical Physics, 1992, 96, 6281-6290.	3.0	18
45	Adsorption of Sodium Dodecyl Sulfate and Butanol onto Acidic and Basic Alumina. Journal of Colloid and Interface Science, 1996, 182, 348-355.	9.4	18
46	Molecular-field splitting and vibrational structure in the phosphorus 2p photoelectron spectrum of PF3. Journal of Chemical Physics, 1999, 111, 4472-4477.	3.0	18
47	First observation of vibrations in core-level photoelectron spectra of free neutral molecular clusters. Chemical Physics Letters, 2006, 429, 109-113.	2.6	18
48	Size of Free Neutral CO₂ Clusters from Carbon 1s Ionization Energies. Journal of Physical Chemistry A, 2011, 115, 10408-10415.	2.5	18
49	2,2â€²-Selenobis(acetic acid), Se(CH 2 C(O)OH) 2 : an old compound with a novel structure. Journal of Molecular Structure, 2000, 554, 149-161.	3.6	16
50	High resolution C1s and S2p photoelectron spectra of thiophene. Journal of Chemical Physics, 2002, 117, 7587-7592.	3.0	16
51	Reduction of chromium in ethylene polymerisation using bis(imido)chromium(vi) catalyst precursorsElectronic supplementary information available: Cartesian coordinate files of the computed stationary points. See http://www.rsc.org/suppdata/cc/b1/b110296f/. Chemical Communications, 2002, , 542-543.	4.1	16
52	Surface relaxation in water clusters: Evidence from theoretical analysis of the oxygen 1s photoelectron spectrum. Journal of Chemical Physics, 2008, 128, 154710.	3.0	16
53	On the cluster-size dependence of electron capture cross sections in ion-cluster collisions. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 25, 247-251.	1.0	15
54	Color and substitution pattern in anthocyanidins. A combined quantum chemicalâ€“chemometrical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 1999, 55, 761-771.	3.9	15

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55	What Can C1s Photoelectron Spectroscopy Tell about Structure and Bonding in Clusters of Methanol and Methyl Chloride?. Journal of Physical Chemistry A, 2007, 111, 8903-8909.	2.5	15
56	Carbon 1s photoelectron spectroscopy of 1-pentyne conformers. Journal of Molecular Structure, 2009, 920, 387-392.	3.6	15
57	The calculation of initial-state effects on inner-shell ionization energies. Journal of Electron Spectroscopy and Related Phenomena, 2000, 107, 155-161.	1.7	14
58	Multiple Additions of Palladium to C60. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 365-371.	2.1	14
59	Laboratory-frame electron angular distributions: Probing the chemical environment through intramolecular electron scattering. Physical Review A, 2013, 87, .	2.5	14
60	Titanium-Ethylene Complexes Proposed To Be Intermediates in Ziegler-Natta Catalysis. Can They Be Detected through Vibrational Spectroscopy?. Organometallics, 1995, 14, 4349-4358.	2.3	12
61	Molecular-field splitting in S2p photoelectron spectra of dimethyl sulfide and sulfur dichloride. Chemical Physics Letters, 1999, 310, 439-444.	2.6	12
62	Structure and Stability of Substitutional Metallofullerenes of the Firstâ€Row Transition Metals. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 269-278.	2.1	12
63	Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne. Journal of Chemical Physics, 2013, 138, 234310.	3.0	12
64	Energy-Dependent Relative Cross Sections in Carbon 1s Photoionization: Separation of Direct Shake and Inelastic Scattering Effects in Single Molecules. Journal of Physical Chemistry A, 2019, 123, 7619-7636.	2.5	12
65	Structure and Stability of Networked Metallofullerenes of the Transition Metals. Journal of Physical Chemistry A, 2006, 110, 11711-11716.	2.5	11
66	Chemical Reactivity of Alkenes and Alkynes As Seen from Activation Energies, Enthalpies of Protonation, and Carbon 1s Ionization Energies. Journal of Organic Chemistry, 2012, 77, 10105-10117.	3.2	11
67	Accurate Enthalpies of Formation for CrX(g), X = O, OH, and F. A Computational Study. Journal of Physical Chemistry A, 1997, 101, 9449-9456.	2.5	9
68	Molecular-field splitting of the 2p3/2 peak in x-ray photoelectron spectra of second-row atoms: A theoretical study of phosphine and phosphorus trifluoride. Journal of Chemical Physics, 1999, 111, 4478-4486.	3.0	9
69	Vibrationally resolved photoelectron spectra of the carbon 1s and nitrogen 1s shells in hydrogen cyanide. Chemical Physics, 2002, 277, 83-90.	1.9	9
70	Franck-Condon transitions in a system with large-amplitude anharmonic vibrations coupled to a harmonic-oscillator bath: Application to the C1sphotoelectron spectrum of ethanol. Physical Review A, 2006, 74, .	2.5	9
71	Neutral CH3Cl and CH3Br clusters studied by X-ray photoelectron spectroscopy and modeling: Insight to intermolecular interactions and structure. Journal of Electron Spectroscopy and Related Phenomena, 2008, 166-167, 53-64.	1.7	9
72	The structure of mixed methanol/chloroform clusters from core-level photoelectron spectroscopy and modeling. New Journal of Chemistry, 2011, 35, 2564.	2.8	8

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73	Accurate metalâ€“ligand bond energies in the Î·²-C₂H₄ and Î·²-C₆₀ complexes of Pt(PH₃)₂, with application to their Bis(triphenylphosphine) analogues. Molecular Physics, 2013, 111, 1599-1611.	1.7	8
74	Conformations and CH/Ï€ Interactions in Aliphatic Alkynes and Alkenes. Journal of Physical Chemistry A, 2013, 117, 2007-2019.	2.5	8
75	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	3.3	8
76	A note on the electronic structure of O 2 ?. Theoretica Chimica Acta, 1990, 77, 409-413.	0.8	7
77	An investigation of the quantum chemical description of the ethylenic double bond in reactions. I. The electrophilic addition of hydrochloric acid to ethylene. Journal of Chemical Physics, 1996, 105, 6910-6920.	3.0	7
78	Two size regimes of methanol clusters produced by adiabatic expansion. Journal of Chemical Physics, 2006, 125, 184303.	3.0	7
79	Structure of Neutral Nanosized Clusters Produced by Coexpansion of CF₄ and CH₄. Journal of Physical Chemistry A, 2011, 115, 13259-13268.	2.5	6
80	Molecular Spectra As a Tool in Assigning Carbon 1s Photoelectron Spectra of Physisorbed Overlayers. Journal of Physical Chemistry C, 2010, 114, 15383-15393.	3.1	5
81	Carbon 1s photoelectron spectroscopy of the chlorinated methanes: Lifetimes and accurate vibrational lineshape models. Journal of Electron Spectroscopy and Related Phenomena, 2012, 185, 226-233.	1.7	5
82	Structure of Self-Assembled Free Methanol/Tetrachloromethane Clusters. Journal of Physical Chemistry A, 2013, 117, 13127-13137.	2.5	5
83	Electronic Properties of Chlorine, Methyl, and Chloromethyl as Substituents to the Ethylene Groupâ€”Viewed from the Core of Carbon. Journal of Physical Chemistry A, 2015, 119, 9481-9493.	2.5	5
84	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	3.3	4
85	Adsorption of Short Chain Alcohols from Decane Solutions onto Kaolinite. Journal of Colloid and Interface Science, 1995, 171, 261-269.	9.4	3
86	Chemisorption of 1,1-dichloroethene on the Si(1 1 1)-7 Ã— 7 surface. Surface Science, 2007, 601, 5510-5514.	1.9	3
87	Valence photoionization and photoelectronâ€“photoion coincidence (PEPICO) study of molecular LiCl and Li2Cl2. Journal of Electron Spectroscopy and Related Phenomena, 2012, 185, 285-293.	1.7	3
88	Effective attenuation length from core-level photoelectron spectroscopy of CS₂clusters. Journal of Physics B: Atomic, Molecular and Optical Physics, 2013, 46, 025102.	1.5	3
89	Electron attenuation in free, neutral ethane clusters. Journal of Chemical Physics, 2014, 141, 164305.	3.0	3
90	X-ray induced fragmentation of size-selected salt cluster-ions stored in an ion trap. RSC Advances, 2014, 4, 47743-47751.	3.6	3

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91	HCl Dissociation in Methanol Clusters from Ab Initio Molecular Dynamics Simulations and Inner-Shell Photoelectron Spectroscopy. Journal of Physical Chemistry A, 2014, 118, 6900-6907.	2.5	3
92	Formation and Growth of Clusters of Sulfur Dioxide. Aerosol Science and Technology, 2015, 49, 451-462.	3.1	2
93	Changing role of carrier gas in formation of ethanol clusters by adiabatic expansion. Journal of Chemical Physics, 2017, 147, 014301.	3.0	2
94	Attenuation of slow (10â€“40 eV) electrons in soft nanoparticles: Size matters in argon clusters. Physical Review E, 2018, 97, 012604.	2.1	2
95	Carbocation stability as predictor for electrophilic addition of HCl to chlorinated ethenes and propenes in the gas phase. Journal of Physical Organic Chemistry, 2019, 32, e3922.	1.9	2
96	Calibration of oxygen 1s ionization energies. Accurate energies for CO2, H2O, CO, and O2. Journal of Electron Spectroscopy and Related Phenomena, 2021, 251, 147103.	1.7	2
97	Theoretical cluster-model study of line-broadening effects in core-level spectra. Physical Review B, 1991, 43, 9413-9419.	3.2	1
98	Electron capture from the light noble gases. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, L677-L683.	1.5	1
99	Second-order MÃ¸llerâ€“Plesset perturbation theory for computing molecular-field splitting: application to the S2p3/2 level in C2H2n+1SF5, n=0, 1, and 2. Chemical Physics, 2001, 270, 55-65.	1.9	1
100	Conductivity studies in benzotrifluoride. Journal of Molecular Liquids, 2003, 103-104, 221-233.	4.9	1
101	Selective vibrational excitation in the resonant Auger decay following core-to- transitions in. Journal of Electron Spectroscopy and Related Phenomena, 2010, 181, 129-134.	1.7	1
102	Comment on â€˜Photoelectron and electron momentum spectroscopy of 1-butene at benchmark theoretical levelsâ€™. Journal of Physics B: Atomic, Molecular and Optical Physics, 2012, 45, 238001.	1.5	1
103	Theoretical Models of Active Sites: General Considerations and Application to the Study of Phillips-Type Cr/Silica Catalysts for Ethylene Polymerization. Nanostructure Science and Technology, 2005, , 85-111.	0.1	1