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	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
2	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
3	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
4	Attenuation of slow (10â€“40 eV) electrons in soft nanoparticles: Size matters in argon clusters. Physical Review E, 2018, 97, 012604.	2.1	2
5	Changing role of carrier gas in formation of ethanol clusters by adiabatic expansion. Journal of Chemical Physics, 2017, 147, 014301.	3.0	2
6	Formation and Growth of Clusters of Sulfur Dioxide. Aerosol Science and Technology, 2015, 49, 451-462.	3.1	2
7	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
8	Electron attenuation in free, neutral ethane clusters. Journal of Chemical Physics, 2014, 141, 164305.	3.0	3
9	X-ray induced fragmentation of size-selected salt cluster-ions stored in an ion trap. RSC Advances, 2014, 4, 47743-47751.	3.6	3
10	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
11	Laboratory-frame electron angular distributions: Probing the chemical environment through intramolecular electron scattering. Physical Review A, 2013, 87, .	2.5	14
12	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
13	Conformations and CH/Ï€ Interactions in Aliphatic Alkynes and Alkenes. Journal of Physical Chemistry A, 2013, 117, 2007-2019.	2.5	8
14	Structure of Self-Assembled Free Methanol/Tetrachloromethane Clusters. Journal of Physical Chemistry A, 2013, 117, 13127-13137.	2.5	5
15	Intensity oscillations in the carbon 1s ionization cross sections of 2-butyne. Journal of Chemical Physics, 2013, 138, 234310.	3.0	12
16	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
17	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
18	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

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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	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
21	Nonstoichiometric Intensities in Core Photoelectron Spectroscopy. Physical Review Letters, 2012, 108, 193005.	7.8	51
22	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
23	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
24	Size of Free Neutral CO₂ Clusters from Carbon 1s Ionization Energies. Journal of Physical Chemistry A, 2011, 115, 10408-10415.	2.5	18
25	Structure of Neutral Nanosized Clusters Produced by Coexpansion of CF₄ and CH₄. Journal of Physical Chemistry A, 2011, 115, 13259-13268.	2.5	6
26	The structure of mixed methanol/chloroform clusters from core-level photoelectron spectroscopy and modeling. New Journal of Chemistry, 2011, 35, 2564.	2.8	8
27	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
28	Chemical shifts of carbon 1s ionization energies. Journal of Electron Spectroscopy and Related Phenomena, 2011, 183, 2-9.	1.7	21
29	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
30	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
31	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
32	Carbon 1s photoelectron spectroscopy of 1-pentyne conformers. Journal of Molecular Structure, 2009, 920, 387-392.	3.6	15
33	Additivity of Substituent Effects. Core-Ionization Energies and Substituent Effects in Fluoromethylbenzenes. Journal of Physical Chemistry A, 2009, 113, 3481-3490.	2.5	23
34	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
35	The O 1s photoelectron spectrum of molecular oxygen revisited. Journal of Physics B: Atomic, Molecular and Optical Physics, 2008, 41, 095101.	1.5	20
36	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

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37	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
38	Effects of molecular conformation on inner-shell ionization energies. Physical Chemistry Chemical Physics, 2007, 9, 719-724.	2.8	22
39	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
40	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
41	Chemisorption of 1,1-dichloroethene on the Si(1 1 1)-7 Ã— 7 surface. Surface Science, 2007, 601, 5510-5514.	1.9	3
42	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
43	Two size regimes of methanol clusters produced by adiabatic expansion. Journal of Chemical Physics, 2006, 125, 184303.	3.0	7
44	Size of neutral argon clusters from core-level photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2006, 8, 1891-1898.	2.8	34
45	Lineshapes in carbon 1s photoelectron spectra of methanol clusters. Physical Chemistry Chemical Physics, 2006, 8, 2473-2482.	2.8	23
46	Structure and Stability of Networked Metallofullerenes of the Transition Metals. Journal of Physical Chemistry A, 2006, 110, 11711-11716.	2.5	11
47	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
48	First observation of vibrations in core-level photoelectron spectra of free neutral molecular clusters. Chemical Physics Letters, 2006, 429, 109-113.	2.6	18
49	Structure and Stability of Substitutional Metallofullerenes of the Firstâ€Row Transition Metals. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 269-278.	2.1	12
50	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
51	Multiple Additions of Palladium to C60. Fullerenes Nanotubes and Carbon Nanostructures, 2006, 14, 365-371.	2.1	14
52	Conformational Effects in Inner-Shell Photoelectron Spectroscopy of Ethanol. Physical Review Letters, 2005, 95, 103002.	7.8	35
53	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
54	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

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55	Catalytic dehydrogenation of ethane over mononuclear Cr(III) surface sites on silica. part I. Câ€”H activation by Ïƒâ€bond metathesis. Journal of Physical Organic Chemistry, 2004, 17, 990-1006.	1.9	44
56	Carbon 1s photoelectron spectroscopy of six-membered cyclic hydrocarbons. Physical Chemistry Chemical Physics, 2004, 6, 4254-4259.	2.8	28
57	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
58	Conductivity studies in benzotrifluoride. Journal of Molecular Liquids, 2003, 103-104, 221-233.	4.9	1
59	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
60	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
61	High resolution C1s and S2p photoelectron spectra of thiophene. Journal of Chemical Physics, 2002, 117, 7587-7592.	3.0	16
62	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
63	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
64	Vibrationally resolved photoelectron spectra of the carbon 1s and nitrogen 1s shells in hydrogen cyanide. Chemical Physics, 2002, 277, 83-90.	1.9	9
65	Theoretical Analysis of CO Adsorption on the Reduced Cr/Silica System. Journal of Catalysis, 2002, 205, 177-190.	6.2	32
66	Molecular-Level Insight into Cr/Silica Phillips-Type Catalysts: Polymerization-Active Mononuclear Chromium Sites. Journal of Catalysis, 2002, 205, 366-374.	6.2	64
67	Molecular-Level Insight into Cr/Silica Phillips-Type Catalysts: Polymerization-Active Dinuclear Chromium Sites. Journal of Catalysis, 2002, 206, 331-338.	6.2	70
68	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
69	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
70	Theoretical Investigation of Bis(imido)chromium(VI) Cations as Polymerization Catalysts. Organometallics, 2001, 20, 616-626.	2.3	24
71	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
72	Theoretical Analysis of dâ€“d Transitions for the Reduced Cr/Silica System. Catalysis Letters, 2001, 75, 49-54.	2.6	32

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73	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
74	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
75	Theoretical Models of Ethylene Polymerization over a Mononuclear Chromium(II)/Silica Site. Journal of Catalysis, 2000, 195, 125-139.	6.2	81
76	Evidence of Fermi resonance in core-ionized methane. Journal of Chemical Physics, 2000, 112, 7986-7991.	3.0	23
77	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
78	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
79	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
80	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
81	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
82	Molecular-field splitting in S2p photoelectron spectra of dimethyl sulfide and sulfur dichloride. Chemical Physics Letters, 1999, 310, 439-444.	2.6	12
83	Molecular adsorption of methane and methyl onto MgO(100) An embedded-cluster study. Surface Science, 1999, 421, 296-307.	1.9	22
84	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
85	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
86	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
87	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
88	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
89	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	3.3	4
90	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

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91	On the calculation of molecular field splitting in S 2p photoelectron spectra. Chemical Physics Letters, 1996, 262, 801-806.	2.6	26
92	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
93	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
94	Use of multivariate methods in the analysis of calculated reaction pathways. Journal of Computational Chemistry, 1996, 17, 1197-1216.	3.3	8
95	Adsorption of Short Chain Alcohols from Decane Solutions onto Kaolinite. Journal of Colloid and Interface Science, 1995, 171, 261-269.	9.4	3
96	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
97	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
98	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
99	Electron capture from the light noble gases. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, L677-L683.	1.5	1
100	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
101	Methane dissociation on a nonplanar MgO(001) surface. Theoretical modeling of surface defects. Journal of Chemical Physics, 1991, 95, 4626-4631.	3.0	39
102	Theoretical cluster-model study of line-broadening effects in core-level spectra. Physical Review B, 1991, 43, 9413-9419.	3.2	1
103	A note on the electronic structure of O 2 ?. Theoretica Chimica Acta, 1990, 77, 409-413.	0.8	7