Alfred Karpfen

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/11504945/publications.pdf

Version: 2024-02-01

89 papers	3,776 citations	81743 39 h-index	133063 59 g-index
89 all docs	89 docs citations	89 times ranked	2412 citing authors

#	Article	IF	Citations
1	Single-Bond Torsional Potentials in Conjugated Systems:â€‰ A Comparison of ab Initio and Density Functional Results. Journal of Physical Chemistry A, 1997, 101, 7426-7433.	1.1	254
2	Molecular Geometries and Vibrational Spectra of Phenol, Benzaldehyde, and Salicylaldehyde:Â Experimental versus Quantum Chemical Data. Journal of Physical Chemistry A, 1997, 101, 2254-2263.	1.1	162
3	The effects of electron correlation on the degree of bond alternation and electronic structure of oligomers of polyacetylene. Journal of Chemical Physics, 1997, 107, 6712-6721.	1.2	143
4	Ab initio studies on polymers. V. Allâ€transâ€polyethylene. Journal of Chemical Physics, 1981, 75, 238-245.	1.2	115
5	Coupled pair functional study on the hydrogen fluoride dimer. I. Energy surface and characterization of stationary points. Chemical Physics, 1988, 121, 137-153.	0.9	102
6	Intramolecular Hydrogen Bonding in 2-Hydroxybenzoyl Compounds:Â Infrared Spectra and Quantum Chemical Calculations. The Journal of Physical Chemistry, 1996, 100, 7418-7425.	2.9	100
7	Ab initio Studies on polymers. Theoretica Chimica Acta, 1979, 53, 65-74.	0.9	94
8	An analytical sixâ€dimensional potential energy surface for (HF)2 from ab initio calculations. Journal of Chemical Physics, 1988, 89, 3002-3007.	1.2	87
9	Charge-Transfer Complexes between NH3and the Halogens F2, ClF, and Cl2:Â An ab Initio Study on the Intermolecular Interaction. Journal of Physical Chemistry A, 2000, 104, 6871-6879.	1.1	85
10	Ab initio studies on hydrogen-bonded clusters. I. Linear and cyclic oligomers of hydrogen cyanide. Chemical Physics, 1987, 113, 53-64.	0.9	83
11	Ab initio studies on heterocyclic conjugated polymers: structure and vibrational spectra of thiophene, oligothiophenes and polythiophene. Computational and Theoretical Chemistry, 1992, 259, 181-198.	1.5	83
12	The intermolecular interaction in the charge-transfer complexes between amines and halogens: A theoretical characterization of the trends in halogen bonding. Theoretical Chemistry Accounts, 2003, 110, 1-9.	0.5	77
13	Ab initio calculations on the excited states of Ï€-systems. I. Valence excitations in acetylene. Chemical Physics, 1986, 102, 77-89.	0.9	73
14	Ab initio studies on heterocyclic conjugated polymers: Structure and vibrational spectra of pyrrole, oligopyrroles, and polypyrrole. Journal of Chemical Physics, 1992, 96, 4464-4473.	1.2	70
15	Blue-Shifted Hydrogen-Bonded Complexes CF3Hâ‹¯(HF)1â‰nâ‰3. Journal of Physical Chemistry A, 2003, 107, 9724-9729.	1.1	69
16	Ab initio studies on infinite linear hydrogen fluoride chains. Chemical Physics Letters, 1976, 44, 459-464.	1.2	68
17	An ab initio calculation of the intramolecular stretching spectra for the HF dimer and its Dâ€substituted isotopic species. Journal of Chemical Physics, 1990, 93, 6266-6280.	1.2	68
18	Cooperative Effects in Hydrogen Bonding. Advances in Chemical Physics, 2003, , 469-510.	0.3	65

#	Article	IF	Citations
19	Theoretical Characterization of the Trends in Halogen Bonding. , 2007, , 1-15.		64
20	An ab initio calculation of the stretching energies for the HF dimer. Journal of Chemical Physics, 1990, 92, 7432-7440.	1.2	62
21	An ab initio semirigid bender calculation of the rotation and transâ€tunneling spectra of (HF)2 and (DF)2. Journal of Chemical Physics, 1989, 91, 5154-5159.	1.2	59
22	Strongly Blue-Shifted Câˆ'H Stretches:Â Interaction of Formaldehyde with Hydrogen Fluoride Clusters. Journal of Physical Chemistry A, 2005, 109, 8930-8937.	1.1	58
23	On blue shifts of Câ€"H stretching modes of dimethyl ether in hydrogen- and halogen-bonded complexes. Chemical Physics Letters, 2006, 431, 428-433.	1.2	58
24	An ab initio study of the hydrogen chloride dimer: The potential energy surface and the characterization of the stationary points. Chemical Physics, 1991, 149, 299-309.	0.9	57
25	Molecular and Electronic Structures of Heteroaromatic Oligomers:Â Model Compounds of Polymers with Quantum-Well Structures. Journal of Organic Chemistry, 1998, 63, 1041-1048.	1.7	57
26	NMR Shieldings in Benzoyl and 2-Hydroxybenzoyl Compounds. Experimental versus GIAO Calculated Data. Journal of Physical Chemistry A, 1997, 101, 9610-9617.	1.1	54
27	Linear and Cyclic Clusters of Hydrogen Cyanide and Cyanoacetylene:Â A Comparative ab Initio and Density Functional Study on Cooperative Hydrogen Bonding. The Journal of Physical Chemistry, 1996, 100, 13474-13486.	2.9	52
28	Limitations of current density functional theories for the description of partial Ï€-bond breaking. Chemical Physics Letters, 1997, 276, 266-268.	1.2	52
29	An analytical ab initio potential surface and the calculated tunneling energies for the HCl dimer. Journal of Molecular Spectroscopy, 1991, 146, 200-219.	0.4	51
30	Blue-shifted hydrogen-bonded complexes. II. CH3Fâ‹¯(HF)1â©½nâ©½3 and CH2F2â‹¯(HF)1â©½nâ©½3. Chemical Physics, 2005, 310 77-84.	0.9	51
31	Convergence problem inab initio crystal orbital calculations. International Journal of Quantum Chemistry, 1981, 19, 1207-1214.	1.0	48
32	Blue-Shifted Aâ€'H Stretching Modes and Cooperative Hydrogen Bonding. 1. Complexes of Substituted Formaldehyde with Cyclic Hydrogen Fluoride and Water Clusters. Journal of Physical Chemistry A, 2007, 111, 8177-8187.	1.1	47
33	Binding mode and free energy prediction of fisetin/β-cyclodextrin inclusion complexes. Beilstein Journal of Organic Chemistry, 2014, 10, 2789-2799.	1.3	47
34	Energy surfaces of hydrogen-bonded complexes in the vapor phase. Topics in Current Chemistry, 1984, , 1-40.	4.0	47
35	The Dimer of Acetylene and the Dimer of Diacetylene:â€‰ A Floppy and a Very Floppy Molecule. Journal of Physical Chemistry A, 1999, 103, 11431-11441.	1.1	46
36	AB initio studies on hydrogen bonded chains. II. Equilibrium geometry and vibrational spectra of the bent chain of hydrogen fluoride molecules. Chemical Physics, 1982, 64, 343-357.	0.9	45

#	Article	IF	Citations
37	Ab initio studies on clusters of polar molecules. stability of cyclic versus open-chain trimers of hydrogen fluoride. Chemical Physics Letters, 1983, 102, 289-291.	1.2	44
38	On the structure of anhydrous Î²-cyclodextrin. Chemical Physics Letters, 2007, 441, 159-162.	1.2	42
39	On the structure and torsional potential of trifluoromethoxybenzene: an ab initio and density functional study. Chemical Physics Letters, 2003, 367, 566-575.	1.2	41
40	Linear versus cyclic (HCN)3: An ab initio study on structure, vibrational spectra, and infrared intensities. Journal of Chemical Physics, 1990, 92, 2469-2477.	1.2	40
41	From butadiene to polyacetylene: An ab initio study on the vibrational spectra of polyenes. Journal of Chemical Physics, 1992, 96, 982-996.	1.2	40
42	Hydrogen bonding in long chains of hydrogen fluoride and long chains and large clusters of water molecules. Theoretica Chimica Acta, 1974, 34, 115-127.	0.9	37
43	Ab initio studies on hydrogen-bonded clusters: Structure and vibrational spectra of cyclic (HF)n complexes. International Journal of Quantum Chemistry, 1990, 38, 129-140.	1.0	37
44	Theoretical force-field model for blue-shifted hydrogen bonds with fluoromethanes. Chemical Physics, 2006, 329, 313-328.	0.9	37
45	Ab initio studies on hydrogen bonded chains. I. Equilibrium geometry of the infinite, linear chain of hydrogen fluoride molecules. Chemical Physics, 1980, 47, 401-406.	0.9	34
46	Abinitio studies on hydrogen bonded chains. V. The structure of infinite chains of methanol and water molecules. Canadian Journal of Chemistry, 1985, 63, 809-815.	0.6	34
47	On the Intramolecular Origin of the Blue Shift of Aâˆ'H Stretching Frequencies: Triatomic Hydrides HAX. Journal of Physical Chemistry A, 2009, 113, 5217-5223.	1.1	33
48	Ab initio studies on hydrogen-bonded chains. III. The linear, infinite chain of hydrogen cyanide molecules. Chemical Physics, 1983, 79, 211-218.	0.9	32
49	Cryospectroscopic and ab initio studies of haloformâ€"trimethylamine H-bonded complexes. Physical Chemistry Chemical Physics, 2009, 11, 1551.	1.3	30
50	Accurate torsional potentials in conjugated systems: ab initio and density functional calculations on 1,3-butadiene and monohalogenated butadienes. Molecular Physics, 2004, 102, 819-826.	0.8	29
51	The Torsional Potential of Dimethyl Peroxide:Â Still a Difficult Case for Theory. Journal of Physical Chemistry A, 2002, 106, 438-446.	1.1	27
52	Ab initio studies on hydrogen-bonded chains. IV. Structure and stability of formic acid chains. Chemical Physics, 1984, 88, 415-423.	0.9	26
53	The interaction of fluorosilanes with hydrogen fluoride clusters: strongly blue-shifted hydrogen bonds. Computational and Theoretical Chemistry, 2004, 710, 85-95.	1.5	25
54	Blue-shifted Aâ€"H stretching frequencies in complexes with methanol: the decisive role of intramolecular coupling. Physical Chemistry Chemical Physics, 2011, 13, 14194.	1.3	25

#	Article	IF	Citations
55	Ab Initio Calculations on the Ground State Properties of Polymers. Physica Scripta, 1982, T1, 79-87.	1.2	24
56	Ab initio studies on polymers. VI. Torsional potential in regular polyethylene chains. Journal of Computational Chemistry, 1984, 5, 11-18.	1.5	24
57	Gauche- versus s-cis-butadiene revisited: a molecular dynamics simulation of the Ar matrix effect. Chemical Physics Letters, 1992, 189, 281-286.	1.2	23
58	Ab initio calculations on the excited states of Ï€-systems. II. Valence excitations in diacetylene. Chemical Physics, 1986, 102, 91-102.	0.9	21
59	The interaction of fluoramines, fluorophosphines and fluoroarsines with hydrogen fluoride clusters (HF)n: Model studies on blue-shifted hydrogen bonds. Computational and Theoretical Chemistry, 2005, 757, 203-215.	1.5	20
60	Does the most stable formic acid tetramer have Ï€ stacking or Câ€“Hâ‹¯O interactions?. Journal of Chemical Physics, 2006, 124, 224313.	1.2	20
61	Charge-Transfer Complexes between the Amines (CH3)nNH3-n (n = 0â^'3) and the ClF Molecule:â€‰ An ab Initio and Density Functional Study on the Intermolecular Interaction. Journal of Physical Chemistry A, 2001, 105, 2064-2072.	1.1	19
62	The dimers of glyoxal and acrolein with H2O and HF: Negative intramolecular coupling and blue-shifted Câ€“H stretch. Chemical Physics Letters, 2010, 489, 39-43.	1.2	18
63	Torsional Potentials of Perfluoro-1,3-butadiene and Perfluoro-1,3,5-hexatriene:â€‰ A Comparison of ab Initio and Density Functional Results. Journal of Physical Chemistry A, 1999, 103, 2821-2827.	1.1	16
64	Hydrogen-bonding interaction of methyl-substituted pyridines with thioacetamide: steric hindrance of methyl group. Chemical Physics Letters, 2001, 345, 338-344.	1.2	15
65	Surprisingly regular structureâ€“property relationships between Câ€“O bond distances and methoxy group torsional potentials: An ab initio and density functional study. Computational and Theoretical Chemistry, 2003, 635, 141-150.	1.5	15
66	Modified eneâ€“yne compounds: a novel functional material with nonlinear optical properties. CrystEngComm, 2011, 13, 7194.	1.3	15
67	Ab initionumerical studies on density-matrix asymptotics in extended systems. Physical Review B, 1983, 27, 7583-7588.	1.1	14
68	The intermolecular interaction between amines and F2. An ab initio study. Chemical Physics Letters, 1999, 299, 493-502.	1.2	14
69	How strong is the edge effect in the adsorption of anticancer drugs on a graphene cluster?. Journal of Molecular Modeling, 2016, 22, 85.	0.8	14
70	Ab initio studies on hydrogen-bonded clusters. II. Structures and vibrational spectra of the hydrogen-bonded trimers (HCN)2HF, (HCN2)HCl, (NCH)2OH2 AND (NCH)2NH3. Chemical Physics, 1988, 120, 199-213.	0.9	13
71	Theoretical and experimental approaches to evaluate the intermolecular hydrogen-bonding ability of tertiary amides. Physical Chemistry Chemical Physics, 2001, 3, 1973-1978.	1.3	13
72	On the interaction of propynal with HNO, HF, HCl, H2O, CH3OH, and NH3: Red- and blue-shifting hydrogen bonds and tetrel bonds. Computational and Theoretical Chemistry, 2019, 1160, 1-13.	1.1	12

#	Article	IF	Citations
73	Ab Initio Studies on Cyanoacetylene Oligomers:Â Rings and Chains versus Stacked Clusters. Journal of Physical Chemistry A, 1998, 102, 9286-9296.	1.1	11
74	The intermolecular interaction in the charge-transfer complex between NH3 and F2. A subtle case. Chemical Physics Letters, 2000, 316, 483-488.	1.2	11
75	Homodromic hydrogen bonds in low-energy conformations of single molecule cyclodextrins. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2007, 57, 35-38.	1.6	10
76	Density functional calculations on cyclodextrins. Monatshefte FÃ¼r Chemie, 2008, 139, 363-371.	0.9	10
77	AHâ‹¯Ï€ hydrogen bonding to acetylene and benzene: The role of intramolecular coupling. Computational and Theoretical Chemistry, 2012, 999, 231-238.	1.1	9
78	Ab initio studies on polymers. VII. Polyoxymethylene. Journal of Computational Chemistry, 1984, 5, 19-23.	1.5	8
79	Trends in the Torsional Potentials of Methoxy and Trifluoromethoxy Groups:Â An ab Initio and Density Functional Study on the Structure of para-Substituted Pyridines and Pyridinium Cations. Journal of Physical Chemistry A, 2003, 107, 2362-2368.	1.1	8
80	Trends in the C-C force constants in oligothiophenes: A quantum chemical study. Journal of Molecular Structure, 1995, 349, 417-420.	1.8	7
81	On the potential energy surfaces of dimers formed between trans-glyoxal, trans-acrolein and formaldehyde. Computational and Theoretical Chemistry, 2015, 1061, 60-71.	1.1	7
82	Ab initio studies on polymers: torsional potential in helical sulfur chains. Chemical Physics Letters, 1987, 136, 571-574.	1.2	6
83	AB Initio Studies on the Structure and Phonon Spectra of Simple Polymers. , 1984, , 33-55.		4
84	Ab initio studies on hydrogen-bonded trimers: structure and vibrational spectra of HCN(HF)2 and (HCN)2HF. Computational and Theoretical Chemistry, 1991, 227, 337-350.	1.5	3
85	Systematic investigation on the binding of GW420867X as HIV-1 reverse transcriptase inhibitor. Monatshefte FÃ¼r Chemie, 2011, 142, 961-971.	0.9	3
86	On the structure of the H 2 CO-HNO dimer: Planar or orthogonal?. Computational and Theoretical Chemistry, 2017, 1108, 10-17.	1.1	2
87	On the interaction of cyanoformaldehyde with HNO, HF, HCl, H 2 O, and CH 3 OH: A preference for orthogonal structures. Computational and Theoretical Chemistry, 2017, 1120, 34-45.	1.1	1
88	The Concept of Molecular Shape Response Quantified within Force Field Approach. AIP Conference Proceedings, 2007, , .	0.3	0
89	The Dimer of Cyanodiacetylene: Stacking vs. Hydrogen Bonding. , 1999, , 73-86.		0