Per-Olof Ãstrand

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8801057/publications.pdf

Version: 2024-02-01

111 papers	4,378 citations	109264 35 h-index	110317 64 g-index
112 all docs	112 docs citations	112 times ranked	3478 citing authors

#	Article	IF	Citations
1	Investigation of the temperature dependence of dielectric relaxation in liquid water by THz reflection spectroscopy and molecular dynamics simulation. Journal of Chemical Physics, 1997, 107, 5319-5331.	1.2	539
2	THz Spectroscopy of LiquidH2OandD2O. Physical Review Letters, 1999, 82, 2888-2891.	2.9	349
3	An efficient approach for calculating vibrational wave functions and zero-point vibrational corrections to molecular properties of polyatomic molecules. Journal of Chemical Physics, 2000, 112, 2668-2683.	1.2	209
4	Polarizability of molecular clusters as calculated by a dipole interaction model. Journal of Chemical Physics, 2002, 116, 4001-4010.	1.2	180
5	Accurate Intermolecular Potentials Obtained from Molecular Wave Functions:â€‰ Bridging the Gap between Quantum Chemistry and Molecular Simulations. Chemical Reviews, 2000, 100, 4087-4108.	23.0	164
6	Zero-Point Vibrational Effects on Proton Shieldings:Â Functional-Group Contributions from ab Initio Calculations. Journal of the American Chemical Society, 2001, 123, 4826-4833.	6.6	127
7	Ab Initio Calculation of the Electronic Spectrum of Azobenzene Dyes and Its Impact on the Design of Optical Data Storage Materials. Journal of the American Chemical Society, 2000, 122, 3482-3487.	6.6	114
8	Calculation of the vibrational wave function of polyatomic molecules. Journal of Chemical Physics, 2000, 112, 2655-2667.	1.2	104
9	Novel model for calculating the intermolecular part of the infrared spectrum for molecular complexes. Journal of Chemical Physics, 1995, 102, 3534-3554.	1.2	95
10	Zero-point vibrational effects on optical rotation. Chemical Physics Letters, 2001, 337, 217-223.	1.2	95
11	Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets. Journal of Physical Chemistry A, 2008, 112, 1392-1402.	1.1	80
12	Nonempirical intermolecular potentials for ureaâ€“water systems. Journal of Chemical Physics, 1994, 100, 1262-1273.	1.2	79
13	Solvent effects on the nâ†'Ï€[sup â^—] electronic transition in formaldehyde: A combined coupled cluster/molecular dynamics study. Journal of Chemical Physics, 2004, 121, 8435.	1.2	75
14	Properties of ureaâ€“water solvation calculated from a newabinitiopolarizable intermolecular potential. Journal of Chemical Physics, 1991, 95, 8419-8429.	1.2	70
15	Static and Frequency-Dependent Polarizability Tensors for Carbon Nanotubes. Journal of Physical Chemistry B, 2000, 104, 10462-10466.	1.2	64
16	Molecular dynamics study of water adopting a potential function with explicit atomic dipole moments and anisotropic polarizabilities. Chemical Physics, 1995, 191, 195-202.	0.9	63
17	Complex formation between water and formamide. Journal of Chemical Physics, 1993, 99, 4894-4907.	1.2	61
18	Frequency-Dependent Molecular Polarizability Calculated within an Interaction Model. Journal of Physical Chemistry A, 2000, 104, 1563-1569.	1.1	60

#	Article	IF	Citations
19	Rovibrationally averaged magnetizability, rotational g factor, and indirect spinâ€“spin coupling of the hydrogen fluoride molecule. Journal of Chemical Physics, 1999, 110, 9463-9468.	1.2	59
20	Solvent effects on nuclear shieldings and spinâ€“spin couplings of hydrogen selenide. Journal of Chemical Physics, 1998, 108, 2528-2537.	1.2	58
21	Chemical Shifts in Liquid Water Calculated by Molecular Dynamics Simulations and Shielding Polarizabilities. Journal of Physical Chemistry B, 1997, 101, 4105-4110.	1.2	57
22	Five-membered rings as diazo components in optical data storage devices: an ab initio investigation of the lowest singlet excitation energies. Chemical Physics Letters, 2000, 325, 115-119.	1.2	57
23	Statistical mechanically averaged molecular properties of liquid water calculated using the combined coupled cluster/molecular dynamics method. Journal of Chemical Physics, 2006, 124, 124503.	1.2	55
24	Effects of additives on prebreakdown phenomena in liquid cyclohexane: II. Streamer propagation. Journal Physics D: Applied Physics, 2007, 40, 5624-5634.	1.3	54
25	Atomic Charges of the Water Molecule and the Water Dimer. Journal of Physical Chemistry A, 1998, 102, 7686-7691.	1.1	51
26	Intermolecular Potential for the 1,2-Dimethoxyethaneâ^'Water Complex. The Journal of Physical Chemistry, 1996, 100, 6950-6957.	2.9	50
27	Field dependence on the molecular ionization potential and excitation energies compared to conductivity models for insulation materials at high electric fields. Journal of Applied Physics, 2011, 109, .	1.1	50
28	A Dipole Interaction Model for the Molecular Second Hyperpolarizability. Journal of Physical Chemistry A, 2003, 107, 2270-2276.	1.1	43
29	Effects of additives on prebreakdown phenomena in liquid cyclohexane: I. Streamer initiation. Journal Physics D: Applied Physics, 2007, 40, 5161-5169.	1.3	43
30	Frequency-Dependent Polarizability of Boron Nitride Nanotubes:Â A Theoretical Study. Journal of Physical Chemistry B, 2001, 105, 10243-10248.	1.2	42
31	Liquid densities and structural properties of molecular models of water. Journal of Chemical Physics, 1995, 102, 6559-6565.	1.2	41
32	Analysis of the conformation of worm-like chains by small-angle scattering: Monte-Carlo simulations in comparison to analytical theory. Macromolecular Theory and Simulations, 2000, 9, 345-353.	0.6	41
33	The Static Polarizability and Second Hyperpolarizability of Fullerenes and Carbon Nanotubesâ€. Journal of Physical Chemistry A, 2004, 108, 8795-8800.	1.1	41
34	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	0.5	38
35	Calculation of nuclear shielding constants and magnetizabilities of the hydrogen fluoride molecule. Journal of Chemical Physics, 1996, 104, 648-653.	1.2	37
36	A Chargeâ^'Dipole Model for the Static Polarizability of Nanostructures Including Aliphatic, Olephinic, and Aromatic Systems. Journal of Physical Chemistry A, 2008, 112, 1277-1285.	1.1	36

#	Article	IF	Citations
37	Excitation energies and ionization potentials at high electric fields for molecules relevant for electrically insulating liquids. Journal of Applied Physics, 2013, 113, .	1.1	36
38	An atomic capacitance-polarizability model for the calculation of molecular dipole moments and polarizabilities. International Journal of Quantum Chemistry, 2001, 84, 513-522.	1.0	34
39	Density Functional Theory Study on the Interactions of Metal Ions with Long Chain Deprotonated Carboxylic Acids. Journal of Physical Chemistry A, 2015, 119, 10195-10203.	1.1	33
40	Magnetizabilities and Nuclear Shielding Constants of the Fluoromethanes in the Gas Phase and Solution. The Journal of Physical Chemistry, 1996, 100, 19771-19782.	2.9	32
41	Saturation of the Third-Order Polarizability of Carbon Nanotubes Characterized by a Dipole Interaction Model. Nano Letters, 2003, 3, 661-665.	4.5	32
42	Microscopic and Macroscopic Polarization in C60 Fullerene Clusters as Calculated by an Electrostatic Interaction Model. Journal of Physical Chemistry B, 2004, 108, 8226-8233.	1.2	31
43	Molecular Dynamics Simulations of Carbon-Supported Ni Clusters Using the Reax Reactive Force Field. Journal of Physical Chemistry C, 2008, 112, 12663-12668.	1.5	28
44	Nonmetallic electronegativity equalization and point-dipole interaction model including exchange interactions for molecular dipole moments and polarizabilities. Journal of Chemical Physics, 2009, 131, 044101.	1.2	28
45	Zero-point vibrational contributions to fluorine shieldings in organic molecules. Physical Chemistry Chemical Physics, 2003, 5, 5015-5020.	1.3	27
46	Electric field-gradient contributions to the chemical shifts of liquid water. Journal of Chemical Physics, 1997, 106, 8332-8338.	1.2	26
47	Frequency-Dependent Molecular Polarizability and Refractive Index:Â Are Substituent Contributions Additive?. Journal of Physical Chemistry A, 1999, 103, 1818-1821.	1.1	25
48	Molecular Dynamics Simulations of Metal Clusters Supported on Fishbone Carbon Nanofibers. Journal of Physical Chemistry C, 2010, 114, 3522-3530.	1.5	24
49	Local polarizability calculations with localized orbitals in the uncoupled Hartree-Fock approximation. Molecular Physics, 1992, 77, 143-155.	0.8	23
50	Quantitative structure-property relationship modeling of GrÃtzel solar cell dyes. Journal of Computational Chemistry, 2014, 35, 214-226.	1.5	23
51	Tuning the Electronic Properties of Single-Atom Pt Catalysts by Functionalization of the Carbon Support Material. Journal of Physical Chemistry C, 2017, 121, 20802-20812.	1.5	23
52	Influence of Carbon Support on Electronic Structure and Catalytic Activity of Pt Catalysts: Binding to the CO Molecule. Journal of Physical Chemistry C, 2016, 120, 12452-12462.	1.5	22
53	An electrostatic interaction model for frequency-dependent polarizability: methodology and applications to hydrocarbons and fullerenes. Nanotechnology, 2008, 19, 025203.	1.3	21
54	Field-dependent molecular ionization and excitation energies: Implications for electrically insulating liquids. AIP Advances, 2014, 4, .	0.6	21

#	Article	IF	Citations
55	Optical Rotation from Coupled Cluster and Density Functional Theory: The Role of Basis Set Convergence. Journal of Chemical Theory and Computation, 2016, 12, 535-548.	2.3	21
56	The inclusion of electron correlation in intermolecular potentials: applications to the formamide dimer and liquid formamide. Theoretical Chemistry Accounts, 2000, 105, 7-14.	0.5	20
57	Frequency-Dependent Polarizabilities of Amino Acids as Calculated by an Electrostatic Interaction Model. Journal of Chemical Theory and Computation, 2005, 1, 626-633.	2.3	20
58	Evolution of Carbon Nanofiber-Supported Pt Nanoparticles of Different Particle Sizes: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2014, 118, 23711-23722.	1.5	19
59	A test on reactive force fields for the study of silica dimerization reactions. Journal of Chemical Physics, 2015, 143, 184113.	1.2	19
60	Molecular Magnetizabilities:Â Zero-Point Vibrational Effects and the Breakdown of Pascal's Rule. Journal of Physical Chemistry A, 2001, 105, 9926-9930.	1.1	18
61	Full CI calculations of the magnetizability and rotational g factor of the hydrogen molecule. Computational and Theoretical Chemistry, 1996, 388, 231-235.	1.5	17
62	Optical Rotation Calculations for a Set of Pyrrole Compounds. Journal of Physical Chemistry A, 2016, 120, 7351-7360.	1.1	17
63	Quantitative prediction of the absorption maxima of azobenzene dyes from bond lengths and critical points in the electron density. Physical Chemistry Chemical Physics, 2007, 9, 2226-2233.	1.3	16
64	A bound HClâ˜' species: an ab initio quantum-chemical study. Chemical Physics Letters, 1990, 175, 624-628.	1.2	15
65	Calculation of the Geometry of the Water Molecule in Liquid Water. Journal of Physical Chemistry A, 1997, 101, 10039-10044.	1.1	15
66	The magnetizability anisotropy and rotational g factor of deuterium hydride and the deuterium molecule. Chemical Physics Letters, 1997, 271, 163-166.	1.2	14
67	Field-dependent ionisation potential by constrained density functional theory. Molecular Physics, 2013, 111, 1456-1461.	0.8	14
68	Local electric field factors by a combined charge-transfer and pointâ€“dipole interaction model. RSC Advances, 2015, 5, 31594-31605.	1.7	13
69	Ab initio calculations on 2-imidazolyl-2-thiazolyl azo compounds â€“ an investigation of potential near-infrared absorbing structures. Chemical Physics Letters, 2001, 343, 171-177.	1.2	12
70	Combined nonmetallic electronegativity equalisation and pointâ€“dipole interaction model for the frequency-dependent polarisability. Molecular Physics, 2013, 111, 1470-1481.	0.8	12
71	Lithium Ionâ€“Water Clusters in Strong Electric Fields: A Quantum Chemical Study. Journal of Physical Chemistry A, 2015, 119, 4983-4992.	1.1	12
72	Electric and magnetic properties of the nitroethene molecule. Molecular Physics, 1997, 92, 89-96.	0.8	11

#	Article	IF	Citations
73	Complex Frequency-Dependent Polarizability through the Ï€ â†' Ï€* Excitation Energy of Azobenzene Molecules by a Combined Charge-Transfer and Point-Dipole Interaction Model. Journal of Physical Chemistry A, 2014, 118, 11282-11292.	1.1	11
74	Structural and electronic properties of the Pt_nâ€"PAH complex (n = 1, 2) from density functional calculations. Physical Chemistry Chemical Physics, 2014, 16, 18586-18595.	1.3	11
75	Thermo-molecular orientation effects in fluids of dipolar dumbbells. Physical Chemistry Chemical Physics, 2014, 16, 22097-22106.	1.3	11
76	Effects of N,N-dimethylaniline and trichloroethene on prebreakdown phenomena in liquid and solid N-tridecane. IEEE Transactions on Dielectrics and Electrical Insulation, 2011, 18, 1886-1896.	1.8	10
77	N-tridecane as a model system for polyethylene: comparison of pre-breakdown phenomena in liquid and solid phase stressed by a fast transient. IEEE Transactions on Dielectrics and Electrical Insulation, 2011, 18, 1929-1946.	1.8	10
78	Evolution of Pt Nanoparticles Supported on Fishbone-Type Carbon Nanofibers with Coneâ€"Helix Structures: A Molecular Dynamics Study. Journal of Physical Chemistry C, 2013, 117, 14261-14271.	1.5	10
79	Solvent Effects on Optical Rotation: On the Balance between Hydrogen Bonding and Shifts in Dihedral Angles. Journal of Physical Chemistry A, 2017, 121, 4765-4777.	1.1	10
80	Chemical Bonding and Electronic Properties of the Co Adatom and Dimer Interacting with Polyaromatic Hydrocarbons. Journal of Physical Chemistry C, 2015, 119, 24425-24438.	1.5	9
81	Local Field Factors and Dielectric Properties of Liquid Benzene. Journal of Physical Chemistry B, 2015, 119, 11839-11845.	1.2	9
82	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. Journal of Physical Chemistry A, 2016, 120, 7973-7986.	1.1	9
83	Atomic magnetizability tensors of benzene and fluoro- and chlorobenzenes. Magnetic Resonance in Chemistry, 1998, 36, 92-97.	1.1	8
84	An investigation of descriptors based on the critical points in the electron density by building quantitative structureâ€"property relationships for proton chemical shifts. Computational and Theoretical Chemistry, 2007, 810, 15-24.	1.5	8
85	First-principles calculations of C diffusion through the surface and subsurface of Ag/Ni(100) and reconstructed Ag/Ni(100). Surface Science, 2010, 604, 186-195.	0.8	8
86	Adsorption of a single Pt atom on polyaromatic hydrocarbons from first-principle calculations. Chemical Physics Letters, 2013, 575, 76-80.	1.2	8
87	Intermolecular interactions of urea and water. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1991, 88, 2457-2464.	0.2	8
88	Molecular Mechanics Interaction Models for Optical Electronic Properties. Journal of Computational and Theoretical Nanoscience, 2009, 6, 270-291.	0.4	7
89	Refractive Index of Liquid Water in Different Solvent Models. Journal of Physical Chemistry A, 2005, 109, 905-914.	1.1	6
90	Validation of critical points in the electron density as descriptors by building quantitative structure-property relationships for the atomic polar tensor. Journal of Computational Chemistry, 2007, 28, 2130-2139.	1.5	6

#	Article	IF	Citations
91	Geometrical flexibility of platinum nanoclusters: impacts on catalytic decomposition of ethylene glycol. Physical Chemistry Chemical Physics, 2017, 19, 28596-28603.	1.3	6
92	Conductivity and capacitance of streamers in avalanche model for streamer propagation in dielectric liquids. Plasma Research Express, 2019, 1, 035014.	0.4	6
93	A comparison of effective and polarizable intermolecular potentials in simulations: liquid water as a test case. Molecular Physics, 2001, 99, 335-348.	0.8	5
94	Vibrational Effects on Molecular Properties in Large Molecules. Journal of Computational Methods in Sciences and Engineering, 2003, 3, 7-39.	0.1	5
95	Atomic dipole moments calculated using analytical molecular second-moment gradients. Journal of Chemical Physics, 2004, 120, 10368-10378.	1.2	5
96	Photoionization model for streamer propagation mode change in simulation model for streamers in dielectric liquids. Plasma Research Express, 2020, 2, 015002.	0.4	5
97	Dynamical Model for SN2 Reactions in Microsolution: The Cl- + CH3Cl -> CH3 + Cl- Reaction. Molecular Dynamics Simulation of Reaction Clusters.. Acta Chemica Scandinavica, 1999, 53, 1043-1053.	0.7	5
98	New features in McStas, version 1.5. Applied Physics A: Materials Science and Processing, 2002, 74, s1511-s1513.	1.1	4
99	GaussDal: An open source database management system for quantum chemical computations. Computer Physics Communications, 2005, 171, 133-153.	3.0	4
100	Density-functional calculations of field-dependent ionization potentials and excitation energies of aromatic molecules. Chemical Physics, 2015, 447, 22-29.	0.9	4
101	Simulation model for the propagation of second mode streamers in dielectric liquids using the Townsend-Meek criterion. Journal of Physics Communications, 2018, 2, 105007.	0.5	4
102	Polarisation of polar dumbbell fluids in thermal gradients: the importance of the treatment of electrostatic interactions. Molecular Physics, 2016, 114, 3249-3254.	0.8	3
103	Analysis of the conformation of worm-like chains by small-angle scattering: Monte-Carlo simulations in comparison to analytical theory. , 2000, 9, 345.		3
104	Thermal decomposition of cyclohexane by Kinetic Monte Carlo simulations and its relevance to streamer formation. , 2016, , .		2
105	Microscopic polarization in ropes and films of aligned carbon nanotubes. Journal of Computational Methods in Sciences and Engineering, 2007, 6, 353-364.	0.1	1
106	Surface and bulk properties of chromium oxide: Implications for reduction by methane. AIP Conference Proceedings, 2015, , .	0.3	1
107	Cerman: Software for simulating streamer propagation in dielectric liquids based on the Townsendâ€“Meek criterion. Computer Physics Communications, 2021, 265, 107987.	3.0	1
108	Molecular Dynamics Simulation of the Solvation of Benzene Anion. Structural and Dynamic Aspects. The Journal of Physical Chemistry, 1994, 98, 8209-8215.	2.9	0

#	Article	IF	Citations
109	Frequency-dependent local field factors in dielectric liquids by a polarizable force field and molecular dynamics simulations. AIP Conference Proceedings, 2015, , .	0.3	0
110	Molecular mechanics model for electronic polarization. , 2006, , 1200-1203.		0
111	BehÃ¶ver Genealogiska FÃ¶reningen en digital tidskrift?. , 2022, , 101.		0