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	BehÃ¶ver Genealogiska FÃ¶reningen en digital tidskrift?. , 2022, , 101.		0
2	Cerman: Software for simulating streamer propagation in dielectric liquids based on the Townsendâ€“Meek criterion. Computer Physics Communications, 2021, 265, 107987.	3.0	1
3	Photoionization model for streamer propagation mode change in simulation model for streamers in dielectric liquids. Plasma Research Express, 2020, 2, 015002.	0.4	5
4	Conductivity and capacitance of streamers in avalanche model for streamer propagation in dielectric liquids. Plasma Research Express, 2019, 1, 035014.	0.4	6
5	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
6	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
7	Geometrical flexibility of platinum nanoclusters: impacts on catalytic decomposition of ethylene glycol. Physical Chemistry Chemical Physics, 2017, 19, 28596-28603.	1.3	6
8	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
9	Thermal decomposition of cyclohexane by Kinetic Monte Carlo simulations and its relevance to streamer formation. , 2016, , .		2
10	Optical Rotation Calculations for a Set of Pyrrole Compounds. Journal of Physical Chemistry A, 2016, 120, 7351-7360.	1.1	17
11	Optical Rotation Calculations for Fluorinated Alcohols, Amines, Amides, and Esters. Journal of Physical Chemistry A, 2016, 120, 7973-7986.	1.1	9
12	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
13	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
14	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
15	A test on reactive force fields for the study of silica dimerization reactions. Journal of Chemical Physics, 2015, 143, 184113.	1.2	19
16	Surface and bulk properties of chromium oxide: Implications for reduction by methane. AIP Conference Proceedings, 2015, , .	0.3	1
17	Frequency-dependent local field factors in dielectric liquids by a polarizable force field and molecular dynamics simulations. AIP Conference Proceedings, 2015, , .	0.3	0
18	Lithium Ionâ€“Water Clusters in Strong Electric Fields: A Quantum Chemical Study. Journal of Physical Chemistry A, 2015, 119, 4983-4992.	1.1	12

#	Article	IF	Citations
19	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
20	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
21	Local Field Factors and Dielectric Properties of Liquid Benzene. Journal of Physical Chemistry B, 2015, 119, 11839-11845.	1.2	9
22	Local electric field factors by a combined charge-transfer and pointâ€“dipole interaction model. RSC Advances, 2015, 5, 31594-31605.	1.7	13
23	Density-functional calculations of field-dependent ionization potentials and excitation energies of aromatic molecules. Chemical Physics, 2015, 447, 22-29.	0.9	4
24	Field-dependent molecular ionization and excitation energies: Implications for electrically insulating liquids. AIP Advances, 2014, 4, .	0.6	21
25	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
26	Quantitative structure-property relationship modeling of GrÃtzel solar cell dyes. Journal of Computational Chemistry, 2014, 35, 214-226.	1.5	23
27	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
28	Thermo-molecular orientation effects in fluids of dipolar dumbbells. Physical Chemistry Chemical Physics, 2014, 16, 22097-22106.	1.3	11
29	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
30	Combined nonmetallic electronegativity equalisation and pointâ€“dipole interaction model for the frequency-dependent polarisability. Molecular Physics, 2013, 111, 1470-1481.	0.8	12
31	Adsorption of a single Pt atom on polyaromatic hydrocarbons from first-principle calculations. Chemical Physics Letters, 2013, 575, 76-80.	1.2	8
32	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
33	Field-dependent ionisation potential by constrained density functional theory. Molecular Physics, 2013, 111, 1456-1461.	0.8	14
34	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
35	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
36	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

#	Article	IF	Citations
37	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
38	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
39	Molecular Dynamics Simulations of Metal Clusters Supported on Fishbone Carbon Nanofibers. Journal of Physical Chemistry C, 2010, 114, 3522-3530.	1.5	24
40	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
41	Molecular Mechanics Interaction Models for Optical Electronic Properties. Journal of Computational and Theoretical Nanoscience, 2009, 6, 270-291.	0.4	7
42	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
43	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
44	Molecular Dynamics Simulations of the Interactions between Platinum Clusters and Carbon Platelets. Journal of Physical Chemistry A, 2008, 112, 1392-1402.	1.1	80
45	An electrostatic interaction model for frequency-dependent polarizability: methodology and applications to hydrocarbons and fullerenes. Nanotechnology, 2008, 19, 025203.	1.3	21
46	Effects of additives on prebreakdown phenomena in liquid cyclohexane: II. Streamer propagation. Journal Physics D: Applied Physics, 2007, 40, 5624-5634.	1.3	54
47	Effects of additives on prebreakdown phenomena in liquid cyclohexane: I. Streamer initiation. Journal Physics D: Applied Physics, 2007, 40, 5161-5169.	1.3	43
48	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
49	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
50	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
51	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
52	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
53	Molecular mechanics model for electronic polarization. , 2006, , 1200-1203.		0
54	GaussDal: An open source database management system for quantum chemical computations. Computer Physics Communications, 2005, 171, 133-153.	3.0	4

#	Article	IF	Citations
55	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
56	Refractive Index of Liquid Water in Different Solvent Models. Journal of Physical Chemistry A, 2005, 109, 905-914.	1.1	6
57	Atomic dipole moments calculated using analytical molecular second-moment gradients. Journal of Chemical Physics, 2004, 120, 10368-10378.	1.2	5
58	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
59	The Static Polarizability and Second Hyperpolarizability of Fullerenes and Carbon Nanotubesâ€. Journal of Physical Chemistry A, 2004, 108, 8795-8800.	1.1	41
60	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
61	Saturation of the Third-Order Polarizability of Carbon Nanotubes Characterized by a Dipole Interaction Model. Nano Letters, 2003, 3, 661-665.	4.5	32
62	A Dipole Interaction Model for the Molecular Second Hyperpolarizability. Journal of Physical Chemistry A, 2003, 107, 2270-2276.	1.1	43
63	Zero-point vibrational contributions to fluorine shieldings in organic molecules. Physical Chemistry Chemical Physics, 2003, 5, 5015-5020.	1.3	27
64	Vibrational Effects on Molecular Properties in Large Molecules. Journal of Computational Methods in Sciences and Engineering, 2003, 3, 7-39.	0.1	5
65	Polarizability of molecular clusters as calculated by a dipole interaction model. Journal of Chemical Physics, 2002, 116, 4001-4010.	1.2	180
66	New features in McStas, version 1.5. Applied Physics A: Materials Science and Processing, 2002, 74, s1511-s1513.	1.1	4
67	Frequency-Dependent Polarizability of Boron Nitride Nanotubes:Â A Theoretical Study. Journal of Physical Chemistry B, 2001, 105, 10243-10248.	1.2	42
68	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
69	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
70	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
71	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
72	Zero-point vibrational effects on optical rotation. Chemical Physics Letters, 2001, 337, 217-223.	1.2	95

#	Article	IF	Citations
73	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
74	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
75	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
76	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
77	A modified variation-perturbation approach to zero-point vibrational motion. Theoretical Chemistry Accounts, 2000, 103, 365-373.	0.5	38
78	Calculation of the vibrational wave function of polyatomic molecules. Journal of Chemical Physics, 2000, 112, 2655-2667.	1.2	104
79	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
80	Static and Frequency-Dependent Polarizability Tensors for Carbon Nanotubes. Journal of Physical Chemistry B, 2000, 104, 10462-10466.	1.2	64
81	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
82	Frequency-Dependent Molecular Polarizability Calculated within an Interaction Model. Journal of Physical Chemistry A, 2000, 104, 1563-1569.	1.1	60
83	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
84	Analysis of the conformation of worm-like chains by small-angle scattering: Monte-Carlo simulations in comparison to analytical theory. , 2000, 9, 345.		3
85	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
86	Frequency-Dependent Molecular Polarizability and Refractive Index:Â Are Substituent Contributions Additive?. Journal of Physical Chemistry A, 1999, 103, 1818-1821.	1.1	25
87	THz Spectroscopy of LiquidH2OandD2O. Physical Review Letters, 1999, 82, 2888-2891.	2.9	349
88	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
89	Atomic magnetizability tensors of benzene and fluoro- and chlorobenzenes. Magnetic Resonance in Chemistry, 1998, 36, 92-97.	1.1	8
90	Atomic Charges of the Water Molecule and the Water Dimer. Journal of Physical Chemistry A, 1998, 102, 7686-7691.	1.1	51

#	Article	IF	Citations
91	Solvent effects on nuclear shieldings and spinâ€“spin couplings of hydrogen selenide. Journal of Chemical Physics, 1998, 108, 2528-2537.	1.2	58
92	Electric and magnetic properties of the nitroethene molecule. Molecular Physics, 1997, 92, 89-96.	0.8	11
93	Electric field-gradient contributions to the chemical shifts of liquid water. Journal of Chemical Physics, 1997, 106, 8332-8338.	1.2	26
94	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
95	Calculation of the Geometry of the Water Molecule in Liquid Water. Journal of Physical Chemistry A, 1997, 101, 10039-10044.	1.1	15
96	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
97	The magnetizability anisotropy and rotational g factor of deuterium hydride and the deuterium molecule. Chemical Physics Letters, 1997, 271, 163-166.	1.2	14
98	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
99	Calculation of nuclear shielding constants and magnetizabilities of the hydrogen fluoride molecule. Journal of Chemical Physics, 1996, 104, 648-653.	1.2	37
100	Intermolecular Potential for the 1,2-Dimethoxyethaneâ^'Water Complex. The Journal of Physical Chemistry, 1996, 100, 6950-6957.	2.9	50
101	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
102	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
103	Liquid densities and structural properties of molecular models of water. Journal of Chemical Physics, 1995, 102, 6559-6565.	1.2	41
104	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
105	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
106	Nonempirical intermolecular potentials for ureaâ€“water systems. Journal of Chemical Physics, 1994, 100, 1262-1273.	1.2	79
107	Complex formation between water and formamide. Journal of Chemical Physics, 1993, 99, 4894-4907.	1.2	61
108	Local polarizability calculations with localized orbitals in the uncoupled Hartree-Fock approximation. Molecular Physics, 1992, 77, 143-155.	0.8	23

#	Article	IF	Citations
109	Properties of ureaâ€“water solvation calculated from a newabinitiopolarizable intermolecular potential. Journal of Chemical Physics, 1991, 95, 8419-8429.	1.2	70
110	Intermolecular interactions of urea and water. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1991, 88, 2457-2464.	0.2	8
111	A bound HClâ‹¯ species: an ab initio quantum-chemical study. Chemical Physics Letters, 1990, 175, 624-628.	1.2	15