Lars OjamÃ¤e

List of Publications by Year
in descending order

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113	6,623	70961	62479
papers	citations	41 h-index	80 g-index

114	114	114	6392
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Structure of the First Coordination Shell in Liquid Water. Science, 2004, 304, 995-999.	6.0	1,287
2	The inhomogeneous structure of water at ambient conditions. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15214-15218.	3.3	526
3	Modeling Molecular Interactions in Water: From Pairwise to Many-Body Potential Energy Functions. Chemical Reviews, 2016, 116, 7501-7528.	23.0	314
4	Spectroscopic probing of local hydrogen-bonding structures in liquid water. Journal of Physics Condensed Matter, 2002, 14, L213-L219.	0.7	262
5	Li and Na Diffusion in TiO2 from Quantum Chemical Theory versus Electrochemical Experiment. Journal of the American Chemical Society, 1997, 119, 7374-7380.	6.6	220
6	IR and quantum-chemical studies of carboxylic acid and glycine adsorption on rutile TiO2 nanoparticles. Journal of Colloid and Interface Science, 2006, 296, 71-78.	5.0	199
7	Potential models for simulations of the solvated proton in water. Journal of Chemical Physics, 1998, 109, 5547-5564.	1.2	187
8	Graph Theoretical Generation and Analysis of Hydrogen-Bonded Structures with Applications to the Neutral and Protonated Water Cube and Dodecahedral Clusters. Journal of Physical Chemistry A, 1998, 102, 2824-2832.	1.1	182
9	Phosphonic acid adsorption at the TiO2 anatase (101) surface investigated by periodic hybrid HF-DFT computations. Surface Science, 2005, 582, 49-60.	0.8	163
10	Anchor group influence on moleculeâ€“metal oxide interfaces: Periodic hybrid DFT study of pyridine bound to TiO2 via carboxylic and phosphonic acid. Chemical Physics Letters, 2005, 415, 375-380.	1.2	137
11	Ab Initio Study of Cooperativity in Water Chains: Binding Energies and Anharmonic Frequencies. The Journal of Physical Chemistry, 1994, 98, 4271-4282.	2.9	123
12	Theoretical IR Spectra for Water Clusters (H2O)n (n = 6â˜’22, 28, 30) and Identification of Spectral Contributions from Different H-Bond Conformations in Gaseous and Liquid Water. Journal of Physical Chemistry A, 2006, 110, 13388-13393.	1.1	113
13	On the use of graph invariants for efficiently generating hydrogen bond topologies and predicting physical properties of water clusters and ice. Journal of Chemical Physics, 2001, 114, 2527-2540.	1.2	110
14	PES Studies of Ru(dcbpyH2)2(NCS)2Adsorption on Nanostructured ZnO for Solar Cell Applications. Journal of Physical Chemistry B, 2002, 106, 10102-10107.	1.2	106
15	The electronic structure and reflectivity of PEDOT:PSS from density functional theory. Chemical Physics, 2011, 384, 44-51.	0.9	102
16	A theoretical study of water clusters: the relation between hydrogen-bond topology and interaction energy from quantum-chemical computations for clusters with up to 22 molecules. Physical Chemistry Chemical Physics, 2005, 7, 1905-1911.	1.3	99
17	Quantum-Chemical and Force-Field Investigations of Ice Ih:Â Computation of Proton-Ordered Structures and Prediction of Their Lattice Energies. Journal of Physical Chemistry B, 2004, 108, 15856-15864.	1.2	97
18	Comment on "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". Science, 2005, 308, 793a-793a.	6.0	90

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19	Potential energy surfaces and vibrational spectra of H5O2+ and larger hydrated proton complexes. International Journal of Quantum Chemistry, 1995, 56, 657-668.	1.0	89
20	Hydrogen-Bond Topology and the IceVII/VIIIand IceIh/XIProton-Ordering Phase Transitions. Physical Review Letters, 2005, 94, 135701.	2.9	86
21	Dye-Sensitization of the TiO₂ Rutile (110) Surface by Perylene Dyes:â€‰ Quantum-Chemical Periodic B3LYP Computations. Journal of Physical Chemistry C, 2007, 111, 12116-12123.	1.5	84
22	Short H-bonds and spontaneous self-dissociation in (H2O)20: Effects of H-bond topology. Journal of Chemical Physics, 2003, 118, 3583-3588.	1.2	83
23	The electronic structure of free water clusters probed by Auger electron spectroscopy. Journal of Chemical Physics, 2005, 123, 054310.	1.2	80
24	Theoretical characterization of divacancies at the surface and in bulk MgO. Journal of Chemical Physics, 1998, 109, 10984-10995.	1.2	77
25	Periodic Hartreeâ€“Fock study of the adsorption of formic acid on ZnO(1010). Chemical Physics Letters, 2000, 321, 302-308.	1.2	63
26	Mechanical and molecular properties of ice VIII from crystalâ€orbital ab initio calculations. Journal of Chemical Physics, 1994, 100, 2128-2138.	1.2	61
27	Structures of the I-, II- and H-Methane Clathrates and the Iceâ^'Methane Clathrate Phase Transition from Quantum-Chemical Modeling with Force-Field Thermal Corrections. Journal of Physical Chemistry A, 2011, 115, 6169-6176.	1.1	61
28	Electronic interactions between aromatic adsorbates and metal oxide substrates calculated from first principles. Chemical Physics Letters, 2002, 364, 469-474.	1.2	60
29	Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions. Physical Review E, 2006, 73, 056113.	0.8	59
30	A theoretical study of water equilibria: The cluster distribution versus temperature and pressure for (H2O)n, n=1â€“60, and ice. Journal of Chemical Physics, 2009, 131, 134302.	1.2	57
31	ZnO Nanoparticles Functionalized with Organic Acids: An Experimental and Quantum-Chemical Study. Journal of Physical Chemistry C, 2009, 113, 17332-17341.	1.5	54
32	The local structure of protonated water from x-ray absorption and density functional theory. Journal of Chemical Physics, 2006, 124, 194508.	1.2	49
33	On the stability of dense versus cage-shaped water clusters: Quantum-chemical investigations of zero-point energies, free energies, basis-set effects and IR spectra of (H2O)12 and (H2O)20. Chemical Physics Letters, 2006, 418, 361-367.	1.2	49
34	Structural, vibrational and electronic properties of a crystalline hydrate from ab initio periodic Hartreeâ€“Fock calculations. Acta Crystallographica Section B: Structural Science, 1994, 50, 268-279.	1.8	47
35	Structure and vibrational spectra of H[sup +](H[sub 2]O)[sub 8]: Is the excess proton in a symmetrical hydrogen bond?. Journal of Chemical Physics, 2000, 113, 5321.	1.2	47
36	Full Dimensional Quantum Calculations of Vibrational Energies of H5O2+. Journal of Physical Chemistry A, 2003, 107, 7142-7151.	1.1	45

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37	Quantum-chemical studies of metal oxides for photoelectrochemical applications. Advances in Quantum Chemistry, 2002, 41, 203-263.	0.4	44
38	Reply to Soper et al.: Fluctuations in water around a bimodal distribution of local hydrogen-bonded structural motifs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	3.3	44
39	Simulation of band widths in liquid water spectra. The breakdown of the frozen-field approximation. Chemical Physics Letters, 1992, 195, 97-103.	1.2	43
40	Nanocrystalline ruthenium oxide and ruthenium in sensing applications â€“ an experimental and theoretical study. Journal of Nanoparticle Research, 2006, 8, 899-910.	0.8	43
41	Embedded-Cluster Study of Hydrogen Interaction with an Oxygen Vacancy at the Magnesium Oxide Surface. Journal of Physical Chemistry B, 1999, 103, 3872-3876.	1.2	42
42	Topology versus temperature: Thermal behavior of H+(H2O)8 and H+(H2O)16. Journal of Chemical Physics, 2000, 112, 710-716.	1.2	42
43	Quantum chemical prediction of the adsorption conformations and dynamics at HCOOH-covered ZnO(1010) surfaces. International Journal of Quantum Chemistry, 2002, 89, 172-180.	1.0	41
44	Water molecules in different crystal surroundings: Vibrational Oâ€“H frequencies from ab initio calculations. Journal of Chemical Physics, 1992, 96, 9035-9045.	1.2	38
45	The OH stretching frequency in liquid water simulations: the classical error. Chemical Physics Letters, 1992, 191, 500-506.	1.2	36
46	Surface interactions between Y2O3 nanocrystals and organic moleculesâ€”an experimental and quantum-chemical study. Surface Science, 2005, 592, 124-140.	0.8	33
47	Anab initiostudy of the OH stretching frequencies in ice II, ice VIII, and ice IX. Journal of Chemical Physics, 1993, 99, 2917-2928.	1.2	28
48	Surface Effects and Quantum Confinement in Nanosized GaN Clusters: Theoretical Predictions. Journal of Physical Chemistry C, 2008, 112, 13516-13523.	1.5	27
49	Câ€“C Stretching Raman Spectra and Stabilities of Hydrocarbon Molecules in Natural Gas Hydrates: A Quantum Chemical Study. Journal of Physical Chemistry A, 2014, 118, 11641-11651.	1.1	27
50	Towards Biocompatibility of RE2O3 Nanocrystals â^' Water and Organic Molecules Chemisorbed on Gd2O3 and Y2O3 Nanocrystals Studied by Quantum-Chemical Computations. Nano Letters, 2006, 6, 2004-2008.	4.5	26
51	In Situ Activation of an Indium(III) Triazenide Precursor for Epitaxial Growth of Indium Nitride by Atomic Layer Deposition. Chemistry of Materials, 2020, 32, 4481-4489.	3.2	26
52	A comparison of Hartree?Fock, MP2, and DFT results for the HCN dimer and crystal. , 1996, 60, 767-778.		23
53	Clathrate ice sL: a new crystalline phase of ice with ultralow density predicted by first-principles phase diagram computations. Physical Chemistry Chemical Physics, 2018, 20, 8333-8340.	1.3	23
54	Ab Initio Study of Growth Mechanism of 4Hâ€“SiC: Adsorption and Surface Reaction of C₂H₂, C₂H₄, CH₄, and CH₃. Journal of Physical Chemistry C, 2017, 121, 1249-1256.	1.5	22

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55	Theoretical simulation of OH and OD stretching bands of isotopically diluted HDO molecules in aqueous solution. Chemical Physics, 1993, 171, 189-201.	0.9	21
56	CH-Stretching Vibrational Trends in Natural Gas Hydrates Studied by Quantum-Chemical Computations. Journal of Physical Chemistry C, 2015, 119, 17084-17091.	1.5	20
57	Development of SiC-FET methanol sensor. Sensors and Actuators B: Chemical, 2011, 160, 72-78.	4.0	19
58	A model for carbon incorporation from trimethyl gallium in chemical vapor deposition of gallium nitride. Journal of Materials Chemistry C, 2016, 4, 863-871.	2.7	19
59	Time evolution of the CO2 hydrogenation to fuels over Cu-Zr-SBA-15 catalysts. Journal of Catalysis, 2018, 362, 55-64.	3.1	19
60	The Endocyclic Carbon Substituent of Guanidinate and Amidinate Precursors Controlling Atomic Layer Deposition of InN Films. Journal of Physical Chemistry C, 2019, 123, 25691-25700.	1.5	19
61	Nanoparticles for long-term stable, more selective MISiCFET gas sensors. Sensors and Actuators B: Chemical, 2005, 107, 831-838.	4.0	18
62	Raman and IR Spectra of Ice Ih and Ice XI with an Assessment of DFT Methods. Journal of Physical Chemistry B, 2016, 120, 11043-11051.	1.2	18
63	Growth Mechanism of SiC Chemical Vapor Deposition: Adsorption and Surface Reactions of Active Si Species. Journal of Physical Chemistry C, 2018, 122, 648-661.	1.5	18
64	Effects from hydrogen bonds on water structure in (H3O)2[Mo6Cl8X6]Â·yH2O X=Cl (y=7), Br (y=6), or I (y=6). Solid State Sciences, 2002, 4, 1017-1022.	1.5	17
65	An ultralow-density porous ice with the largest internal cavity identified in the water phase diagram. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 12684-12691.	3.3	16
66	From Molecule to Cluster to Bulk: Water OH Vibrations in Different Surroundings. International Journal of Quantum Chemistry, 1992, 42, 1251-1270.	1.0	15
67	Shortcomings of CVD modeling of SiC today. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	15
68	Hexacoordinated Gallium(III) Triazenide Precursor for Epitaxial Gallium Nitride by Atomic Layer Deposition. Chemistry of Materials, 2021, 33, 3266-3275.	3.2	15
69	On the role of electric fields for proton transfer in water. Solid State Ionics, 1995, 77, 34-42.	1.3	14
70	Computational studies of the stability of the (H2O)100 nanodrop. Computational and Theoretical Chemistry, 2010, 944, 163-167.	1.5	14
71	Silicon Chemistry in Fluorinated Chemical Vapor Deposition of Silicon Carbide. Journal of Physical Chemistry C, 2017, 121, 2711-2720.	1.5	14
72	A study of vibrational modes in Na+beta -alumina by molecular dynamics simulation. Journal of Physics Condensed Matter, 1994, 6, 1319-1332.	0.7	13

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73	Growth Mechanism of SiC CVD: Surface Etching by H₂, H Atoms, and HCl. Journal of Physical Chemistry A, 2018, 122, 2503-2512.	1.1	13
74	Kinetic modeling of ammonia decomposition at chemical vapor deposition conditions. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, .	0.9	13
75	Fingerprints in IR OH vibrational spectra of H2O clusters from different H-bond conformations by means of quantum-chemical computations. Journal of Molecular Modeling, 2014, 20, 2281.	0.8	12
76	An investigation of H-atom positions in sulfuric acid crystal structures. Acta Crystallographica Section B: Structural Science, 2004, 60, 179-183.	1.8	11
77	Adsorption and surface diffusion of silicon growth species in silicon carbide chemical vapour deposition processes studied by quantum-chemical computations. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	11
78	On the work function and the charging of small (râ‰ 5â€‰nm) nanoparticles in plasmas. Physics of Plasmas, 2017, 24, .	0.7	11
79	Vibrational Study of SO_x Adsorption on Pt/SiO₂. Journal of Physical Chemistry C, 2014, 118, 29713-29723.	1.5	10
80	Synthesis, Characterization, and Thermal Study of Divalent Germanium, Tin, and Lead Triazenides as Potential Vapor Deposition Precursors. Inorganic Chemistry, 2021, 60, 12759-12765.	1.9	10
81	A Systematic Method for Predictive In Silico Chemical Vapor Deposition. Journal of Physical Chemistry C, 2020, 124, 7725-7736.	1.5	10
82	Quantum-chemical investigations of phenol and larger aromatic molecules at the TiO₂anatase (101) surface. Journal of Physics: Conference Series, 2008, 117, 012020.	0.3	9
83	Brominated Chemistry for Chemical Vapor Deposition of Electronic Grade SiC. Chemistry of Materials, 2015, 27, 793-801.	3.2	9
84	Reduction of Carbon Impurities in Aluminum Nitride from Time-Resolved Chemical Vapor Deposition Using Trimethylaluminum. Journal of Physical Chemistry C, 2020, 124, 14176-14181.	1.5	9
85	SiC-FET methanol sensors for process control and leakage detection. Sensors and Actuators B: Chemical, 2013, 187, 553-562.	4.0	8
86	Synthesis and Thermal Study of Hexacoordinated Aluminum(III) Triazenides for Use in Atomic Layer Deposition. Inorganic Chemistry, 2021, 60, 4578-4587.	1.9	8
87	Controlled CVD Growth of Highly âŸ¨111âŸ©-Oriented 3C-SiC. Journal of Physical Chemistry C, 2022, 126, 9918-9925.	1.5	8
88	Electronic structure effects from hydrogen bonding in the liquid phase and in chemisorption: an integrated theory and experimental effort. Journal of Synchrotron Radiation, 2001, 8, 136-140.	1.0	7
89	Matching precursor kinetics to afford a more robust CVD chemistry: a case study of the C chemistry for silicon carbide using SiF₄ as Si precursor. Journal of Materials Chemistry C, 2017, 5, 5818-5823.	2.7	7
90	Formation of porous ice frameworks at room temperature. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	7

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91	13C Chemical Shift in Natural Gas Hydrates from First-Principles Solid-State NMR Calculations. Journal of Physical Chemistry C, 2016, 120, 1130-1136.	1.5	6
92	Surface Structures from NH₃ Chemisorption in CVD and ALD of AlN, GaN, and InN Films. Journal of Physical Chemistry C, 2022, 126, 5885-5895.	1.5	6
93	The OH stretching frequency in LiClO4Â·3H2O(s) from ab initio and model potential calculations. Chemical Physics, 1992, 161, 87-98.	0.9	5
94	Methylamines as Nitrogen Precursors in Chemical Vapor Deposition of Gallium Nitride. Journal of Physical Chemistry C, 2019, 123, 6701-6710.	1.5	5
95	Understanding indium nitride thin film growth under ALD conditions by atomic scale modelling: From the bulk to the In-rich layer. Applied Surface Science, 2022, 592, 153290.	3.1	5
96	Metal Oxide Nanoparticles as Novel Gate Materials for Field-Effect Gas Sensors. Materials and Manufacturing Processes, 2006, 21, 275-278.	2.7	4
97	Amorphous on the surface. Nature Materials, 2011, 10, 725-726.	13.3	4
98	Simulations of the thermodynamics and kinetics of NH 3 at the RuO 2 (110) surface. Surface Science, 2017, 656, 77-85.	0.8	4
99	Nucleation of titanium nanoparticles in an oxygen-starved environment. II: theory. Journal Physics D: Applied Physics, 2018, 51, 455202.	1.3	4
100	Disorder dynamics in solid 9â€hydroxyphenalenone. Journal of Chemical Physics, 1991, 95, 2696-2701.	1.2	3
101	FET Gas-Sensing Mechanism, Experimental and Theoretical Studies. , 2009, , 1-27.		3
102	On the change of preferential growth orientation in chemical vapor deposition of titanium carbide by aromatic hydrocarbon precursors. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2013, 31, .	0.9	3
103	Thermochemical Properties of Halides and Halohydrides of Silicon and Carbon. ECS Journal of Solid State Science and Technology, 2016, 5, P27-P35.	0.9	3
104	Thermal study of an indium trisguanidinate as a possible indium nitride precursor. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	0.9	3
105	Unprecedented differences in the diamond nucleation density between carbon- and silicon-faces of 4H-silicon carbides. Chinese Chemical Letters, 2020, 31, 2013-2018.	4.8	3
106	SiC based Field Effect Transistor for H<inf>2</inf>S detection. , 2011, , .		2
107	A theoretical study of the electronic structure of GaN nanorods. International Journal of Quantum Chemistry, 2012, 112, 1796-1802.	1.0	2
108	Perspectiveâ€"Current Understanding of the Halogenated Deposition Chemistry for Chemical Vapor Deposition of SiC. ECS Journal of Solid State Science and Technology, 2020, 9, 104006.	0.9	2

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109	Computational study of the catalytic effect of platinum on the decomposition of DNT. International Journal of Quantum Chemistry, 2012, 112, 1852-1858.	1.0	1
110	Revisiting the Thermochemical Database of Si-C-H System Related to SiC CVD Modeling. Materials Science Forum, 0, 778-780, 175-178.	0.3	1
111	Effects from Hydrogen Bonds on Water Structure in (H3O)2[Mo6Cl8X6]Ã—yH2O X: Cl (y = 7), Br (y = 6), or I (y = 6).. ChemInform, 2003, 34, no-no.	0.1	0
112	Full Dimensional Quantum Calculations of Vibrational Energies of H5O+2.. ChemInform, 2003, 34, no.	0.1	0
113	Theoretical Simulation of OH and OD Stretching Bands of Isotopically Diluted HDO Molecules in Lithium Formate Solution. , 1994, , 251-254.		0