Laurence Leherte

List of Publications by Year
in descending order

75 papers	694 citations	687363 13 h-index	794594 19 g-index
81 all docs	81 docs citations	81 times ranked	486 citing authors

#	Article	IF	Citations
1	Determination of the self-diffusion coefficient of water in ferrierite by molecular dynamics. Chemical Physics Letters, 1988, 145, 237-241.	2.6	40
2	Energetics and diffusion of butene isomers in channel zeolites from molecular dynamics simulations. Journal of Molecular Catalysis A, 1997, 119, 165-176.	4.8	29
3	Self-diffusion of water into a ferrierite-type zeolite by molecular dynamics simulations. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1959-1970.	1.7	27
4	Molecular Mechanical Investigation of the Energetics of Butene Sorbed in H-Ferrierite. Molecular Simulation, 1996, 17, 175-196.	2.0	25
5	Analysis of MD Trajectories as a Jump Diffusion Process:â€‰ Butene Isomers in Zeolite Types TON and MEL. Journal of Physical Chemistry B, 1997, 101, 4717-4732.	2.6	24
6	Effects of long-range interactions in zeolite-like systems: interaction energies and self-diffusion coefficient of water in ferrierite from molecular dynamics simulation. Journal of Molecular Catalysis, 1989, 54, 426-438.	1.2	22
7	Molecular Mechanism for the Self-Supported Synthesis of Graphitic Carbon Nitride from Urea Pyrolysis. Journal of Physical Chemistry Letters, 2021, 12, 1396-1406.	4.6	20
8	A New Graph Descriptor for Molecules Containing Cycles. Application as Screening Criterion for Searching Molecular Structures within Large Databases of Organic Compounds. Journal of Chemical Information and Computer Sciences, 2001, 41, 1437-1445.	2.8	19
9	Dynamics of benzene in zeolite KL. Journal of Molecular Catalysis A, 2001, 166, 147-165.	4.8	18
10	Confinement in molecular sieves: The pioneering physical concepts. Journal of Molecular Catalysis A, 2009, 305, 16-23.	4.8	15
11	What does zeolitic water look like?: Modelization by molecular dynamics simulations. International Journal of Quantum Chemistry, 1992, 42, 1291-1326.	2.0	14
12	Shape information from a critical point analysis of calculated electron density maps: Application to DNA-drug systems. Journal of Computer-Aided Molecular Design, 1994, 8, 257-272.	2.9	14
13	Comparison of Benzodiazepine-Like Compounds Using Topological Analysis and Genetic Algorithms. SAR and QSAR in Environmental Research, 1998, 8, 195-232.	2.2	14
14	Critical Point Representations of Electron Density Maps for the Comparison of Benzodiazepine-Type Ligands. Journal of Chemical Information and Computer Sciences, 2000, 40, 816-832.	2.8	14
15	On the Modularity of the Intrinsic Flexibility of the Âμ Opioid Receptor: A Computational Study. PLoS ONE, 2014, 9, e115856.	2.5	14
16	Title is missing!. Journal of Mathematical Chemistry, 2001, 29, 47-83.	1.5	13
17	Analysis of Three-Dimensional Protein Images. Journal of Artificial Intelligence Research, 0, 7, 125-159.	7.0	13
18	Molecular scene analysis: the integration of direct-methods and artificial-intelligence strategies for solving protein crystal structure. Acta Crystallographica Section D: Biological Crystallography, 1993, 49, 168-178.	2.5	12

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19	Parameterization of the ReaxFF reactive force field for a proline-catalyzed aldol reaction. Journal of Computational Chemistry, 2016, 37, 2564-2572.	3.3	12
20	Influence of the presence of the heme cofactor on the JK-loop structure in indoleamine 2,3-dioxygenase 1. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1211-1221.	2.3	12
21	Molecular scene analysis: application of a topogical approach to the automated interpretation of protein electron-density maps. Acta Crystallographica Section D: Biological Crystallography, 1994, 50, 155-166.	2.5	11
22	Evaluation of the protein solvent-accessible surface using reduced representations in terms of critical points of the electron density. Journal of Computational Chemistry, 2004, 25, 1117-1126.	3.3	11
23	Coarse Point Charge Models For Proteins From Smoothed Molecular Electrostatic Potentials. Journal of Chemical Theory and Computation, 2009, 5, 3279-3298.	5.3	11
24	Crystal structures and snapshots along the reaction pathway of human phosphoserine phosphatase. Acta Crystallographica Section D: Structural Biology, 2019, 75, 592-604.	2.3	11
25	Study of the water behavior into a ferrierite zeolite by molecular dynamics simulations. Computers & Chemistry, 1991, 15, 273-285.	1.2	10
26	Molecular dynamics studies of sorbates in zeolites: water in ferrierite. Catalysis Today, 1991, 10, 177-200.	4.4	10
27	Structural Identification of Local Maxima in Low-Resolution Promolecular Electron Density Distributions. Journal of Physical Chemistry A, 2003, 107, 9875-9886.	2.5	10
28	Hierarchical analysis of promolecular full electron-density distributions: description of protein structure fragments. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1254-1265.	2.5	10
29	Influence of conformation on the representation of small flexible molecules at low resolution: alignment of endothiapepsin ligands. Journal of Computer-Aided Molecular Design, 2005, 19, 525-549.	2.9	10
30	Structural, energetic, and dynamical properties of rotaxanes constituted of Î±-cyclodextrins and an azobenzene chain. Journal of Molecular Graphics and Modelling, 2007, 26, 104-116.	2.4	10
31	[8] Critical-point analysis in protein electron-density map interpretation. Methods in Enzymology, 1997, 277, 131-157.	1.0	9
32	Critical Point Analysis of Calculated Electron Density Maps at Medium Resolution: Application to Shape Analysis of Zeolite-Like Systems. Journal of Molecular Modeling, 1997, 3, 156-171.	1.8	9
33	Interaction between probe molecules and zeolites.. Physical Chemistry Chemical Physics, 2002, 4, 2416-2423.	2.8	9
34	Description of proteinâ€“DNA complexes in terms of electron-density topological features. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 2150-2162.	2.5	9
35	Similarity measures based on Gaussian-type promolecular electron density models: Alignment of small rigid molecules. Journal of Computational Chemistry, 2006, 27, 1800-1816.	3.3	9
36	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminiumâ€“enamine conversion in a proline-catalyzed reaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	9

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37	Quantum mechanical investigations on the role of neutral and negatively charged enamine intermediates in organocatalyzed reactions. Chemical Physics, 2014, 434, 30-36.	1.9	9
38	On the origin of an external surface barrier to sorption in microporous solids: Reply to F. Vignï¿½-Maeder. Journal of Catalysis, 1989, 119, 266-268.	6.2	8
39	Use of Electron Density Critical Points as Chemical Function-Based Reduced Representations of Pharmacological Ligands. Journal of Chemical Information and Computer Sciences, 2004, 44, 1394-1401.	2.8	8
40	Topological Analysis of Proteins as Derived from Medium and High-resolution Electron Density: Applications to Electrostatic Properties. , 0, , 285-315.		8
41	Charge density distributions derived from smoothed electrostatic potential functions: design of protein reduced point charge models. Journal of Computer-Aided Molecular Design, 2011, 25, 913-930.	2.9	8
42	Topological analysis of electron density maps of chiral cyclodextrin-guest complexes: a steric interaction evaluation. Supramolecular Science, 1995, 2, 209-217.	0.7	7
43	Similarity and complementarity of molecular shapes: Applicability of a topological analysis approach. Journal of Computer-Aided Molecular Design, 1996, 10, 55-66.	2.9	6
44	Smoothed Gaussian molecular fields: an evaluation of molecular alignment problems. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	6
45	Multiscale design of coarse-grained elastic network-based potentials for the Î¼ opioid receptor. Journal of Molecular Modeling, 2016, 22, 227.	1.8	6
46	Reduced Point Charge Models of Proteins: Effect of Proteinâ€“Water Interactions in Molecular Dynamics Simulations of Ubiquitin Systems. Journal of Physical Chemistry B, 2017, 121, 9771-9784.	2.6	6
47	Interaction of POPC, DPPC, and POPE with the Î¼ opioid receptor: A coarse-grained molecular dynamics study. PLoS ONE, 2019, 14, e0213646.	2.5	6
48	Effects of Long-Range Interactions in Zeolites-Like Systems: Dynamical Behavior of Water in Ferrierite From Molecular Dynamics Simulation. Studies in Surface Science and Catalysis, 1989, , 773-783.	1.5	5
49	Can Descriptors of the Electron Density Distribution Help To Distinguish Functional Groups?. Journal of Chemical Information and Modeling, 2008, 48, 1974-1983.	5.4	5
50	Evaluation of reduced point charge models of proteins through Molecular Dynamics simulations: Application to the Vps27 UIM-1â€“Ubiquitin complex. Journal of Molecular Graphics and Modelling, 2014, 47, 44-61.	2.4	5
51	Investigating cyclic peptides inhibiting CD2â€“CD58 interactions through molecular dynamics and molecular docking methods. Journal of Computer-Aided Molecular Design, 2018, 32, 1295-1313.	2.9	5
52	Development of a Genetic Algorithm Method Especially Designed for the Comparison of Molecular Models: Application to the Elucidation of the Benzodiazepine Receptor Pharmacophore. , 0, , 497-509.		5
53	A Theoretical View and Approach to the Physics and Chemistry of Zeolites and Molecular Sieves. , 1990, , 1-51.		5
54	Monte Carlo Simulations of Water Interaction with a Ferrlerite Type Zeolite Structure. Studies in Surface Science and Catalysis, 1988, , 293-300.	1.5	4

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55	Application of a Kohonen neural network to the analysis of data regarding the alkylation of toluene with methanol catalyzed by ZSM-5 type zeolites. Computers & Chemistry, 2002, 26, 557-572.	1.2	4
56	Comparison of reduced point charge models of proteins: Molecular Dynamics simulations of Ubiquitin. Science China Chemistry, 2014, 57, 1340-1354.	8.2	4
57	Formation and structural, energetic and dynamic properties of cyclodextrin host tubes and included guest molecules. Supramolecular Chemistry, 2015, 27, 90-109.	1.2	4
58	Accessing the free energy profile of a ring closure in a proline-catalyzed reaction using a reactive force field. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	4
59	Collective motions in protein structures: Applications of elastic network models built from electron density distributions. Computer Physics Communications, 2008, 179, 171-180.	7.5	3
60	Collective motions of rigid fragments in protein structures from smoothed electron density distributions. Journal of Computational Chemistry, 2008, 29, 1472-1489.	3.3	3
61	Implementation of a Protein Reduced Point Charge Model toward Molecular Dynamics Applications. Journal of Physical Chemistry A, 2011, 115, 12531-12543.	2.5	3
62	Reduced point charge models of proteins: assessment based on molecular dynamics simulations. Molecular Simulation, 2016, 42, 289-304.	2.0	3
63	Multiresolution non-covalent interaction analysis for ligandâ€“protein promolecular electron density distributions. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
64	Temporary Intermediates of L-Trp Along the Reaction Pathway of Human Indoleamine 2,3-Dioxygenase 1 and Identification of an Exo Site. International Journal of Tryptophan Research, 2021, 14, 117864692110529.	2.3	3
65	Computerised structural analysis of zeolitic networks: Conceptualisation of a zeolite scene through graphs comparison. Journal of Computer-Aided Materials Design, 1994, 1, 265-284.	0.7	2
66	Storing, retrieving, and analyzing experimental catalyticdata with the help of artificial intelligence methods. Studies in Surface Science and Catalysis, 1995, 94, 525-535.	1.5	2
67	Modeling of Structural, Energetic, and Dynamic Properties of Fewâ€Atom Silver Clusters Embedded in Polynucleotide Strands by Using Molecular Dynamics. ChemPhysChem, 2015, 16, 360-369.	2.1	2
68	Structure and Dynamics of an Archeal Monoglyceride Lipase from Palaeococcus ferrophilus as Revealed by Crystallography and In Silico Analysis. Biomolecules, 2021, 11, 533.	4.0	2
69	Linear dependence of the interaction energy on intramolecular distance for adsorbed or clustered diatomic molecules. Molecular Physics, 2000, 98, 1433-1439.	1.7	1
70	Investigation of bound and unbound phosphoserine phosphatase conformations through elastic network models and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 3958-3974.	3.5	1
71	Structure-based identification of inhibitors disrupting the CD2â€“CD58 interactions. Journal of Computer-Aided Molecular Design, 2021, 35, 337-353.	2.9	1
72	Protein-Protein Docking Using Three-Dimensional Reduced Representations and Based on a Genetic Algorithm. , 2008, , 301-323.		1

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73	Molecular graphics applied to the investigations of sorbates in zeolites. , 1993, , 997-1002.		1
74	Use of Electron Density Critical Points as Chemical Function-Based Reduced Representations of Pharmacological Ligands.. ChemInform, 2004, 35, no.	0.0	0
75	Smoothed Gaussian molecular fields: an evaluation of molecular alignment problems. Highlights in Theoretical Chemistry, 2014, , 189-204.	0.0	0