

Matthias Hennemann

List of Publications by Year in descending order

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33
papers

2,935
citations

516215

16
h-index

414034

32
g-index

36
all docs

36
docs citations

36
times ranked

3318
citing authors

#	ARTICLE	IF	CITATIONS
1	Halogen bonding: the σ -hole. <i>Journal of Molecular Modeling</i> , 2007, 13, 291-296.	0.8	2,004
2	Solvatochromic covalent organic frameworks. <i>Nature Communications</i> , 2018, 9, 3802.	5.8	171
3	Polarization-induced σ -holes and hydrogen bonding. <i>Journal of Molecular Modeling</i> , 2012, 18, 2461-2469.	0.8	121
4	Improving the Charge Transport in Self-Assembled Monolayer Field-Effect Transistors: From Theory to Devices. <i>Journal of the American Chemical Society</i> , 2013, 135, 4893-4900.	6.6	72
5	CypScore: Quantitative Prediction of Reactivity toward Cytochromes P450 Based on Semiempirical Molecular Orbital Theory. <i>ChemMedChem</i> , 2009, 4, 657-669.	1.6	69
6	Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal-Organic Framework Architectures. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5519-5526.	7.2	66
7	EMPIRE: a highly parallel semiempirical molecular orbital program: 1: self-consistent field calculations. <i>Journal of Molecular Modeling</i> , 2014, 20, 2331.	0.8	52
8	Solvation Largely Accounts for the Effect of N-Alkylation on the Properties of Nickel(II/I) and Chromium(III/II) Cyclam Complexes. <i>Inorganic Chemistry</i> , 2002, 41, 2927-2935.	1.9	40
9	In Silico Prediction of Buffer Solubility Based on Quantum-Mechanical and HQSAR- and Topology-Based Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 648-658.	2.5	35
10	P6 Manganocene and P3 Cymantrene: Consequences of the Inclusion of Phosphorus Atoms in Mn-Coordinated Cyclopentadienyl Ligands. <i>Angewandte Chemie - International Edition</i> , 2000, 39, 2087-2091.	7.2	33
11	A QSPR-Approach to the Estimation of the pK_{HB} of Six-Membered Nitrogen-Heterocycles using Quantum Mechanically Derived Descriptors. <i>Journal of Molecular Modeling</i> , 2002, 8, 95-101.	0.8	33
12	EMPIRE: a highly parallel semiempirical molecular orbital program: 2: periodic boundary conditions. <i>Journal of Molecular Modeling</i> , 2015, 21, 144.	0.8	27
13	Quantum Mechanics-Based Properties for 3D-QSAR. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1486-1502.	2.5	24
14	An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18065-18072.	7.2	24
15	Ambiphilicity: A Characteristic Reactivity Principle of σ -Bound Phosphorus Heterocycles. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 4047-4052.	7.2	22
16	Near-infrared Fourier transform surface-enhanced Raman scattering spectroscopy of 1,4-benzodiazepine drugs employing gold films over nanospheres. <i>Journal of Raman Spectroscopy</i> , 2004, 35, 368-383.	1.2	16
17	Unprecedented triphosphinine iron interactions: Intramolecular electron transfer, reactivity round a corner, and a low-activated ring element exchange reaction. <i>Comptes Rendus Chimie</i> , 2010, 13, 1203-1212.	0.2	14
18	Predicting the Sites and Energies of Noncovalent Intermolecular Interactions Using Local Properties. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1061-1071.	2.5	14

#	ARTICLE	IF	CITATIONS
19	An ab initio and Density Functional Theory Study of Radical-Clock Reactions. <i>Journal of Organic Chemistry</i> , 2008, 73, 1536-1545.	1.7	13
20	Self-consistent field convergence for proteins: a comparison of full and localized-molecular-orbital schemes. <i>Journal of Molecular Modeling</i> , 2014, 20, 2159.	0.8	12
21	Propagation of Holes and Electrons in Metal-Organic Frameworks. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5057-5064.	2.5	12
22	The hpCADD NDDO Hamiltonian: Parametrization. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1907-1922.	2.5	11
23	EMPIRE: a highly parallel semiempirical molecular orbital program: 3: Born-Oppenheimer molecular dynamics. <i>Journal of Molecular Modeling</i> , 2020, 26, 43.	0.8	10
24	Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal-Organic Framework Architectures. <i>Angewandte Chemie</i> , 2021, 133, 5579-5586.	1.6	8
25	The Effect of a Complexed Lithium Cation on a Norcaradiene-Based Radical Clock. <i>Chemistry - A European Journal</i> , 2009, 15, 2425-2433.	1.7	7
26	Intramolecular Reactivity of π -Coordinated P-Heterocycles: How to Form Five-Membered Rings out of Phosphaalkynes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2002, 177, 1523-1527.	0.8	4
27	Spontaneous butenolide ring formation of pregnane-21-O-malonyl hemiesters under mild reaction conditions is facilitated by the 14 β -hydroxy group present in all natural cardenolides. <i>Tetrahedron</i> , 2016, 72, 4556-4563.	1.0	4
28	Size-Dependent Local Ordering in Melanin Aggregates and Its Implication on Optical Properties. <i>Journal of Physical Chemistry A</i> , 2019, 123, 9403-9412.	1.1	4
29	An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework. <i>Angewandte Chemie</i> , 2021, 133, 18213-18220.	1.6	4
30	Quantum-mechanics-based molecular interaction fields for 3D-QSAR. <i>Journal of Cheminformatics</i> , 2014, 6, O10.	2.8	3
31	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. <i>Journal of Molecular Modeling</i> , 2019, 25, 156.	0.8	3
32	The Feynman dispersion correction for MNDO extended to F, Cl, Br and I. , 2019, 25, 1.		1
33	Titelbild: An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework (Angew.) Tj ETQq1_1_0.784314 rgBT		