

Rochus Schmid

List of Publications by Year in descending order

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109
papers

5,372
citations

76294

40
h-index

88593

70
g-index

135
all docs

135
docs citations

135
times ranked

5896
citing authors

#	ARTICLE	IF	CITATIONS
1	Metal@MOF: Loading of Highly Porous Coordination Polymers Host Lattices by Metal Organic Chemical Vapor Deposition. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 6237-6241.	7.2	662
2	Surface Chemistry of Metal-Organic Frameworks at the Liquid-Solid Interface. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 176-199.	7.2	292
3	Structural Complexity in Metal-Organic Frameworks: Simultaneous Modification of Open Metal Sites and Hierarchical Porosity by Systematic Doping with Defective Linkers. <i>Journal of the American Chemical Society</i> , 2014, 136, 9627-9636.	6.6	240
4	Loading of porous metal-organic open frameworks with organometallic CVD precursors: inclusion compounds of the type [LnM] ₃ @MOF-5. <i>Journal of Materials Chemistry</i> , 2006, 16, 2464-2472.	6.7	204
5	Molecular Dynamics Simulation of Benzene Diffusion in MOF-5: Importance of Lattice Dynamics. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 463-466.	7.2	195
6	A Cryogenically Flexible Covalent Organic Framework for Efficient Hydrogen Isotope Separation by Quantum Sieving. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 13219-13222.	7.2	183
7	MOFFFF - A flexible first-principles derived force field for metal-organic frameworks. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 1128-1141.	0.7	162
8	Pentlandite rocks as sustainable and stable efficient electrocatalysts for hydrogen generation. <i>Nature Communications</i> , 2016, 7, 12269.	5.8	150
9	A novel method to measure diffusion coefficients in porous metal-organic frameworks. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8092.	1.3	141
10	QuickFF: A program for a quick and easy derivation of force fields for metal-organic frameworks from <i>ab initio</i> input. <i>Journal of Computational Chemistry</i> , 2015, 36, 1015-1027.	1.5	132
11	Flexibility and Sorption Selectivity in Rigid Metal-Organic Frameworks: The Impact of Ether-Functionalised Linkers. <i>Chemistry - A European Journal</i> , 2010, 16, 14296-14306.	1.7	128
12	Ab initio parametrized MM3 force field for the metal-organic framework MOF-5. <i>Journal of Computational Chemistry</i> , 2007, 28, 1169-1176.	1.5	112
13	Systematic First Principles Parameterization of Force Fields for Metal-Organic Frameworks using a Genetic Algorithm Approach. <i>Journal of Physical Chemistry B</i> , 2009, 113, 1341-1352.	1.2	102
14	Fe-B Bonding in (Dibromoboryl)ferrocene: A Structural and Theoretical Investigation. <i>Organometallics</i> , 1996, 15, 1188-1194.	1.1	90
15	First-Principles-Derived Force Field for Copper Paddle-Wheel-Based Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2010, 114, 14402-14409.	1.5	85
16	Coordination Chemistry and Mechanisms of Metal-Catalyzed CC-Coupling Reactions. 10. Ligand Dissociation in Rhodium-Catalyzed Hydroformylation: A Theoretical Study. <i>Organometallics</i> , 1997, 16, 701-708.	1.1	77
17	A Molecular Model To Explain and Predict the Stereoselectivity in Rhodium-Catalyzed Hydroformylation. <i>Organometallics</i> , 1998, 17, 2141-2143.	1.1	70
18	Surface Termination of the Metal-Organic Framework HKUST-1: A Theoretical Investigation. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3206-3210.	2.1	65

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19	The [Ga ₂ (C ₅ Me ₅) ₂] ⁺ Ion: Bipyramidal Double-Cone Structure and Weakly Coordinated, Monovalent Ga ⁺ . <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1074-1076.	7.2	64
20	Density Functional Study of the Migratory Insertion Step in the Carbonylation of Methanol Catalyzed by [M(CO) ₂ I ₂]- (M = Rh, Ir). <i>Organometallics</i> , 2000, 19, 1973-1982.	1.1	62
21	Mechanistic Insights into an Unprecedented C-C Bond Activation on a Rh/Ga Bimetallic Complex: A Combined Experimental/Computational Approach. <i>Journal of the American Chemical Society</i> , 2005, 127, 17068-17078.	6.6	58
22	Hypothetical 3D-periodic covalent organic frameworks: exploring the possibilities by a first principles derived force field. <i>CrystEngComm</i> , 2013, 15, 1551.	1.3	57
23	A Combined QM/MM Method for the Determination of Regioselectivities in Rhodium-Catalyzed Hydroformylation. <i>Organometallics</i> , 1998, 17, 4828-4834.	1.1	56
24	An Accurate Force Field Model for the Strain Energy Analysis of the Covalent Organic Framework COF-102. <i>Journal of the American Chemical Society</i> , 2008, 130, 12600-12601.	6.6	56
25	Orbital directing effects in copper and zinc based paddle-wheel metal organic frameworks: the origin of flexibility. <i>Journal of Materials Chemistry</i> , 2012, 22, 10249.	6.7	56
26	Frustrated flexibility in metal-organic frameworks. <i>Nature Communications</i> , 2021, 12, 4097.	5.8	55
27	Prediction of Structure and Properties of Boron-Based Covalent Organic Frameworks by a First-Principles Derived Force Field. <i>Journal of Physical Chemistry C</i> , 2012, 116, 4921-4929.	1.5	52
28	Cycloheptatrienyl-Cyclopentadienyl-Zirconium Sandwich Complexes: Structure and Bonding. <i>Organometallics</i> , 2005, 24, 3163-3171.	1.1	50
29	Conformational Isomerism in the Isoreticular Metal Organic Framework Family: A Force Field Investigation. <i>Journal of Physical Chemistry C</i> , 2008, 112, 14980-14987.	1.5	50
30	CO Adsorption on a Mixed-Valence Ruthenium Metal-Organic Framework Studied by UHV-FTIR Spectroscopy and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2013, 117, 5658-5666.	1.5	48
31	Exploring Network Topologies of Copper Paddle Wheel Based Metal-Organic Frameworks with a First-Principles Derived Force Field. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15133-15139.	1.5	47
32	Molecular Dynamics Simulations of the "Breathing" Phase Transformation of MOF Nanocrystallites. <i>Advanced Theory and Simulations</i> , 2019, 2, 1900117.	1.3	47
33	Atomistic theoretical models for nanoporous hybrid materials. <i>Microporous and Mesoporous Materials</i> , 2010, 129, 304-318.	2.2	46
34	Mechanism of benzene diffusion in MOF-5: A molecular dynamics investigation. <i>Microporous and Mesoporous Materials</i> , 2009, 125, 90-96.	2.2	45
35	Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2420-2432.	2.3	45
36	Structure and Metal Coordination of the Diphosphine 2,2'-Bis((diphenylphosphino)methyl)-1,1'-binaphthyl (NAPHOS). <i>Organometallics</i> , 1995, 14, 1961-1968.	1.1	43

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37	Oberflächenchemie Metall-organischer Gerüststoffe an der Flüssig-fest-Grenzfläche. <i>Angewandte Chemie</i> , 2011, 123, 184-208.	1.6	43
38	Substituent-free Gallium by Hydrogenolysis of Coordinated GaCp*: Synthesis and Structure of Highly Fluxional [Ru ₂ (Ga)(GaCp*) ₇ (H) ₃]. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 3872-3876.	7.2	42
39	Polymerization Catalysts with dnElectrons (n= 1-4): A Theoretical Study. <i>Organometallics</i> , 2000, 19, 2756-2765.	1.1	41
40	Ab initio molecular dynamics with a continuum solvation model. <i>Journal of Chemical Physics</i> , 2003, 118, 1089-1100.	1.2	38
41	Low-temperature CO Oxidation over Cu-based Metal-organic Frameworks Monitored by using FTIR Spectroscopy. <i>ChemCatChem</i> , 2012, 4, 755-759.	1.8	38
42	Advanced buckyball joints: synthesis, complex formation and computational simulations of centrohexasindane-extended tribenzotriquinacene receptors for C ₆₀ fullerene. <i>Dalton Transactions</i> , 2012, 41, 5995.	1.6	36
43	Multiscale Modeling of the HKUST-1/Poly(vinyl alcohol) Interface: From an Atomistic to a Coarse Graining Approach. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21491-21496.	1.5	36
44	Ethylene-polymerization by surface supported Cr(IV) species: possible reaction mechanisms revisited by theoretical calculations. <i>Canadian Journal of Chemistry</i> , 2000, 78, 265-269.	0.6	35
45	A general and efficient pseudopotential Fourier filtering scheme for real space methods using mask functions. <i>Journal of Chemical Physics</i> , 2006, 124, 174102.	1.2	32
46	Coarse graining of force fields for metal-organic frameworks. <i>Dalton Transactions</i> , 2016, 45, 4370-4379.	1.6	32
47	Tribenzotriquinacene Receptors for C ₆₀ ... Fullerene Rotors: Towards Chiral Symmetrical Chiral Stators for Unidirectionally Operating Nanoratchets. <i>Chemistry - A European Journal</i> , 2014, 20, 9100-9110.	1.7	30
48	Isorecticular isomerism in 4,4-connected paddle-wheel metal-organic frameworks: structural prediction by the reverse topological approach. <i>CrystEngComm</i> , 2015, 17, 344-352.	1.3	30
49	Retrofitting metal-organic frameworks. <i>Nature Communications</i> , 2019, 10, 4921.	5.8	30
50	Configurational Entropy Driven High-pressure Behaviour of a Flexible Metal-organic Framework (MOF). <i>Angewandte Chemie - International Edition</i> , 2021, 60, 787-793.	7.2	30
51	Tuning the Electric Field Response of MOFs by Rotatable Dipolar Linkers. <i>ACS Central Science</i> , 2019, 5, 1440-1448.	5.3	28
52	The reaction of RhCp*(CH ₃) ₂ (L) (L = pyridine, dmsO) with GaCp* and AlCp*: A new type of carbon-carbon bond activation reaction. <i>Dalton Transactions</i> , 2004, , 3171-3172.	1.6	27
53	Assessing negative thermal expansion in mesoporous metal-organic frameworks by molecular simulation. <i>Journal of Materials Chemistry A</i> , 2019, 7, 24019-24026.	5.2	27
54	Diiminates and Diamides as Ligands in Polymerization Catalysts with M(III) (M = Ti, V, Cr) Metal Centers. A Theoretical Study. <i>Organometallics</i> , 2000, 19, 3069-3076.	1.1	25

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55	Gas Phase Chemistry in Gallium Nitride CVD: Theoretical Determination of the Arrhenius Parameters for the First Ga-C Bond Homolysis of Trimethylgallium. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2623-2630.	1.1	25
56	Car-Parrinello simulations with a real space method. <i>Journal of Computational Chemistry</i> , 2004, 25, 799-812.	1.5	24
57	TopoFF: MOF structure prediction using specifically optimized blueprints. <i>Faraday Discussions</i> , 2018, 211, 79-101.	1.6	24
58	An Electric Field Induced Breath for Metal-Organic Frameworks. <i>ACS Central Science</i> , 2017, 3, 369-371.	5.3	22
59	A Consistent Force Field for the Carboxylate Group. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2822-2834.	2.3	21
60	Almost Enclosed Buckyball Joints: Synthesis, Complex Formation, and Computational Simulations of Pentacyclic Extended Tribenzotriquinacene. <i>ChemPhysChem</i> , 2014, 15, 3855-3863.	1.0	21
61	The Impact of Mesopores on the Mechanical Stability of HKUST-1: A Multiscale Investigation. <i>European Journal of Inorganic Chemistry</i> , 2016, 2016, 4517-4523.	1.0	21
62	Dioxygen binding to Fe-MOF-74: microscopic insights from periodic QM/MM calculations. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1144-1150.	0.6	21
63	Evaluating Computational Shortcuts in Supercell-Based Phonon Calculations of Molecular Crystals: The Instructive Case of Naphthalene. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2716-2735.	2.3	21
64	Rotational and translational dynamics of CO ₂ adsorbed in MOF Zn ₂ (bdc) ₂ (dabco). <i>Microporous and Mesoporous Materials</i> , 2015, 216, 75-81.	2.2	20
65	Computational Structure Prediction of (4,4)-Connected Copper Paddle-wheel-based MOFs: Influence of Ligand Functionalization on the Topological Preference. <i>Crystal Growth and Design</i> , 2018, 18, 2699-2706.	1.4	16
66	Car-Parrinello molecular dynamics using real space wavefunctions. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 1001-1015.	0.7	15
67	Influence of Pore Dimension on the Host-Guest Interaction in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2016, 120, 27319-27327.	1.5	15
68	Beyond the Scholl reaction - one-step planarization and edge chlorination of nanographenes by mechanochemistry. <i>RSC Advances</i> , 2021, 11, 38026-38032.	1.7	15
69	Materials Chemistry of Group 13 Nitrides. , 0, , 49-80.		14
70	Adsorption of Hydrocarbons in Metal-Organic Frameworks: A Force Field Benchmark on the Example of Benzene in Metal-Organic Framework 5. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15369-15377.	1.5	14
71	Model Study of Thermoresponsive Behavior of Metal-Organic Frameworks Modulated by Linker Functionalization. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6835-6841.	1.5	14
72	Electrode potential dependent desolvation and resolvation of germanium(100) in contact with aqueous perchlorate electrolytes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13585-13595.	1.3	14

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73	Identifying the Bottleneck for Heat Transport in Metal-Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2021, 4, 2000211.	1.3	14
74	Calculation of rotational partition functions by an efficient Monte Carlo importance sampling technique. <i>Journal of Computational Chemistry</i> , 2005, 26, 1579-1591.	1.5	13
75	Molecular Dynamics Investigation of the Dielectric Decrement of Ion Solutions. <i>ChemElectroChem</i> , 2018, 5, 1444-1450.	1.7	13
76	Influence of biomass torrefaction parameters on fast pyrolysis products under flame-equivalent conditions. <i>Biomass and Bioenergy</i> , 2018, 119, 392-410.	2.9	13
77	Molecular Insight into the Swelling of a MOF: A Force-Field Investigation of Methanol Uptake in MIL-88B(Fe)-Cl. <i>Journal of Physical Chemistry C</i> , 2021, 125, 12837-12847.	1.5	13
78	The [Ga ₂ (C ₅ Me ₅) ₂] ⁺ Ion: Bipyramidal Double-Cone Structure and Weakly Coordinated, Monovalent Ga ⁺ . <i>Angewandte Chemie - International Edition</i> , 2006, 45, 1674-1674.	7.2	12
79	Influence of flexible side-chains on the breathing phase transition of pillared layer MOFs: a force field investigation. <i>Faraday Discussions</i> , 2021, 225, 324-340.	1.6	12
80	Theoretical Investigation of the Gas-Phase Decomposition of Ga(N ₃) ₂ Et as a Model for a Single-Molecule GaN Precursor. <i>Chemical Vapor Deposition</i> , 2003, 9, 272-278.	1.4	11
81	A parallel multigrid accelerated Poisson solver for ab initio molecular dynamics applications. <i>Computing and Visualization in Science</i> , 2008, 11, 115-122.	1.2	11
82	NMR studies of benzene mobility in metal-organic framework MOF-5. <i>EPJ Applied Physics</i> , 2011, 55, 20702.	0.3	11
83	Rhodium-Catalyzed <i>ortho</i> -Arylation of (Hetero)aromatic Acids. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 3925-3929.	2.1	11
84	Photochemical Sandmeyer-Type Halogenation of Arenediazonium Salts. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	11
85	Solution of high order compact discretized 3D elliptic partial differential equations by an accelerated multigrid method. <i>Journal of Computational and Applied Mathematics</i> , 2019, 350, 343-352.	1.1	10
86	A Multiscale Simulation Approach for the MOCVD of GaN Using a Single-Molecule Precursor in a Vertical Stagnation Flow Reactor. <i>Chemical Vapor Deposition</i> , 2005, 11, 306-316.	1.4	9
87	Experimental Evidence for the Incorporation of Two Metals at Equivalent Lattice Positions in Mixed-Metal Metal-Organic Frameworks. <i>Chemistry - A European Journal</i> , 2020, 26, 5667-5675.	1.7	9
88	Configurational Entropy Driven High-Pressure Behaviour of a Flexible Metal-Organic Framework (MOF). <i>Angewandte Chemie</i> , 2021, 133, 800-806.	1.6	9
89	Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9626-9637.	1.1	8
90	Molecular Dynamics Simulations of the Breathing Phase Transition of MOF Nanocrystallites II: Explicitly Modeling the Pressure Medium. <i>Frontiers in Chemistry</i> , 2021, 9, 757680.	1.8	8

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91	Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach. <i>Energy & Fuels</i> , 2021, 35, 1535-1545.	2.5	8
92	Thermodynamic Stability of Small GaN _n Clusters as Intermediates in GaN CVD. <i>Chemical Vapor Deposition</i> , 2007, 13, 84-90.	1.4	6
93	Linking Fluid Densimetry and Molecular Simulation: Adsorption Behavior of Carbon Dioxide on Planar Gold Surfaces. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 13283-13289.	1.8	6
94	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. <i>Journal of Computational Chemistry</i> , 2021, 42, 2264-2282.	1.5	6
95	Ferrocene in the metal-organic framework MOF-5 studied by homo- and heteronuclear correlation NMR and MD simulation. <i>Microporous and Mesoporous Materials</i> , 2014, 186, 130-136.	2.2	5
96	Exploring the Impact of the Linker Length on Heat Transport in Metal-Organic Frameworks. <i>Nanomaterials</i> , 2022, 12, 2142.	1.9	5
97	Development of a MOF-FF-compatible interaction model for liquid methanol and Cl ⁻ in methanol. <i>Journal of Molecular Liquids</i> , 2019, 285, 526-534.	2.3	4
98	Structure searching methods: general discussion. <i>Faraday Discussions</i> , 2018, 211, 133-180.	1.6	3
99	Theoretical determination of accurate rate constants: Application to the decomposition of a single-molecule precursor. <i>Surface and Coatings Technology</i> , 2007, 201, 8818-8824.	2.2	2
100	Advanced characterisation techniques: multi-scale, <i>in situ</i> , and time-resolved: general discussion. <i>Faraday Discussions</i> , 2021, 225, 152-167.	1.6	2
101	Innenrücktitelbild: Configurational Entropy Driven High-Pressure Behaviour of a Flexible Metal-Organic Framework (MOF) (Angew. Chem. 2/2021). <i>Angewandte Chemie</i> , 2021, 133, 1047-1047.	1.6	2
102	High Order Compact Multigrid Solver for Implicit Solvation Models. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1293-1301.	2.3	1
103	Novel computational tools: general discussion. <i>Faraday Discussions</i> , 2021, 225, 341-357.	1.6	1
104	Ab initio molecular dynamics simulations of the ferroelectric-paraelectric phase transition in sodium nitrite. <i>Physical Review Materials</i> , 2019, 3, .	0.9	1
105	Cover Picture: Substituent-Free Gallium by Hydrogenolysis of Coordinated GaCp*: Synthesis and Structure of Highly Fluxional [Ru ₂ (Ga)(GaCp*) ₇ (H) ₃] (<i>Angew. Chem. Int. Ed.</i> 21/2009). <i>Angewandte Chemie - International Edition</i> , 2009, 48, 3713-3713.	7.2	0
106	Verlet-like algorithms for Car-Parrinello molecular dynamics with unequal electronic occupations. <i>Journal of Chemical Physics</i> , 2017, 147, 114102.	1.2	0
107	Materials breaking the rules: general discussion. <i>Faraday Discussions</i> , 2021, 225, 255-270.	1.6	0
108	(Invited) Understanding Phonons and Thermal Transport in Metal-Organic Frameworks. <i>ECS Meeting Abstracts</i> , 2020, MA2020-02, 2019-2019.	0.0	0

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109	MD Studies of Methanol Confined in the Metal-Organic Framework MOF MIL-88B-Cl. Journal of Molecular Liquids, 2022, , 119252.	2.3	0