Rochus Schmid

List of Publications by Year
in descending order

109	5,372	76294	88593
papers	citations	40 h-index	70 g-index

135	135	135	5896
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Photochemical Sandmeyerâ€type Halogenation of Arenediazonium Salts. Chemistry - A European Journal, 2022, 28, .	1.7	11
2	MD Studies of Methanol Confined in the Metal-Organic Framework MOF MIL-88B-Cl. Journal of Molecular Liquids, 2022, , 119252.	2.3	0
3	Exploring the Impact of the Linker Length on Heat Transport in Metalâ€“Organic Frameworks. Nanomaterials, 2022, 12, 2142.	1.9	5
4	Influence of flexible side-chains on the breathing phase transition of pillared layer MOFs: a force field investigation. Faraday Discussions, 2021, 225, 324-340.	1.6	12
5	Configurational Entropy Driven Highâ€Pressure Behaviour of a Flexible Metalâ€“Organic Framework (MOF). Angewandte Chemie, 2021, 133, 800-806.	1.6	9
6	Identifying the Bottleneck for Heat Transport in Metalâ€“Organic Frameworks. Advanced Theory and Simulations, 2021, 4, 2000211.	1.3	14
7	Configurational Entropy Driven Highâ€Pressure Behaviour of a Flexible Metalâ€“Organic Framework (MOF). Angewandte Chemie - International Edition, 2021, 60, 787-793.	7.2	30
8	Advanced characterisation techniques: multi-scale, in situ, and time-resolved: general discussion. Faraday Discussions, 2021, 225, 152-167.	1.6	2
9	Molecular Insight into the Swelling of a MOF: A Force-Field Investigation of Methanol Uptake in MIL-88B(Fe)â€“Cl. Journal of Physical Chemistry C, 2021, 125, 12837-12847.	1.5	13
10	Frustrated flexibility in metal-organic frameworks. Nature Communications, 2021, 12, 4097.	5.8	55
11	Materials breaking the rules: general discussion. Faraday Discussions, 2021, 225, 255-270.	1.6	0
12	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
13	InnenrÃ¼cktitelbild: Configurational Entropy Driven Highâ€Pressure Behaviour of a Flexible Metalâ€“Organic Framework (MOF) (Angew. Chem. 2/2021). Angewandte Chemie, 2021, 133, 1047-1047.	1.6	2
14	Molecular Dynamics Simulations of the Breathing Phase Transition of MOF Nanocrystallites II: Explicitly Modeling the Pressure Medium. Frontiers in Chemistry, 2021, 9, 757680.	1.8	8
15	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. Journal of Computational Chemistry, 2021, 42, 2264-2282.	1.5	6
16	Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach. Energy & Fuels, 2021, 35, 1535-1545.	2.5	8
17	Beyond the Scholl reaction â€“ one-step planarization and edge chlorination of nanographenes by mechanochemistry. RSC Advances, 2021, 11, 38026-38032.	1.7	15
18	Experimental Evidence for the Incorporation of Two Metals at Equivalent Lattice Positions in Mixedâ€Metal Metalâ€“Organic Frameworks. Chemistry - A European Journal, 2020, 26, 5667-5675.	1.7	9

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19	Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. Journal of Physical Chemistry A, 2020, 124, 9626-9637.	1.1	8
20	Linking Fluid Densimetry and Molecular Simulation: Adsorption Behavior of Carbon Dioxide on Planar Gold Surfaces. Industrial & Engineering Chemistry Research, 2020, 59, 13283-13289.	1.8	6
21	Evaluating Computational Shortcuts in Supercell-Based Phonon Calculations of Molecular Crystals: The Instructive Case of Naphthalene. Journal of Chemical Theory and Computation, 2020, 16, 2716-2735.	2.3	21
22	(Invited) Understanding Phonons and Thermal Transport in Metal-Organic Frameworks. ECS Meeting Abstracts, 2020, MA2020-02, 2019-2019.	0.0	0
23	Tuning the Electric Field Response of MOFs by Rotatable Dipolar Linkers. ACS Central Science, 2019, 5, 1440-1448.	5.3	28
24	Retrofitting metal-organic frameworks. Nature Communications, 2019, 10, 4921.	5.8	30
25	Molecular Dynamics Simulations of the â€œBreathingâ€•Phase Transformation of MOF Nanocrystallites. Advanced Theory and Simulations, 2019, 2, 1900117.	1.3	47
26	Assessing negative thermal expansion in mesoporous metalâ€“organic frameworks by molecular simulation. Journal of Materials Chemistry A, 2019, 7, 24019-24026.	5.2	27
27	Rhodiumâ€Catalyzed orthoâ€Arylation of (Hetero)aromatic Acids. Advanced Synthesis and Catalysis, 2019, 361, 3925-3929.	2.1	11
28	Development of a MOF-FF-compatible interaction model for liquid methanol and Clâ¯ in methanol. Journal of Molecular Liquids, 2019, 285, 526-534.	2.3	4
29	Ab Initio Derived Force Fields for Zeolitic Imidazolate Frameworks: MOF-FF for ZIFs. Journal of Chemical Theory and Computation, 2019, 15, 2420-2432.	2.3	45
30	Solution of high order compact discretized 3D elliptic partial differential equations by an accelerated multigrid method. Journal of Computational and Applied Mathematics, 2019, 350, 343-352.	1.1	10
31	High Order Compact Multigrid Solver for Implicit Solvation Models. Journal of Chemical Theory and Computation, 2019, 15, 1293-1301.	2.3	1
32	Ab initio molecular dynamics simulations of the ferroelectric-paraelectric phase transition in sodium nitrite. Physical Review Materials, 2019, 3, .	0.9	1
33	Molecular Dynamics Investigation of the Dielectric Decrement of Ion Solutions. ChemElectroChem, 2018, 5, 1444-1450.	1.7	13
34	Computational Structure Prediction of (4,4)-Connected Copper Paddle-wheel-based MOFs: Influence of Ligand Functionalization on the Topological Preference. Crystal Growth and Design, 2018, 18, 2699-2706.	1.4	16
35	TopoFF: MOF structure prediction using specifically optimized blueprints. Faraday Discussions, 2018, 211, 79-101.	1.6	24
36	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	1.6	3

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37	Influence of biomass torrefaction parameters on fast pyrolysis products under flame-equivalent conditions. Biomass and Bioenergy, 2018, 119, 392-410.	2.9	13
38	An Electric Field Induced Breath for Metalâ€“Organic Frameworks. ACS Central Science, 2017, 3, 369-371.	5.3	22
39	Electrode potential dependent desolvation and resolvation of germanium(100) in contact with aqueous perchlorate electrolytes. Physical Chemistry Chemical Physics, 2017, 19, 13585-13595.	1.3	14
40	Verlet-like algorithms for Car-Parrinello molecular dynamics with unequal electronic occupations. Journal of Chemical Physics, 2017, 147, 114102.	1.2	0
41	Multiscale Modeling of the HKUST-1/Poly(vinyl alcohol) Interface: From an Atomistic to a Coarse Graining Approach. Journal of Physical Chemistry C, 2017, 121, 21491-21496.	1.5	36
42	The Impact of Mesopores on the Mechanical Stability of HKUSTâ€1: A Multiscale Investigation. European Journal of Inorganic Chemistry, 2016, 2016, 4517-4523.	1.0	21
43	Influence of Pore Dimension on the Hostâ€“Guest Interaction in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 27319-27327.	1.5	15
44	Dioxygen binding to Fe-MOF-74: microscopic insights from periodic QM/MM calculations. Canadian Journal of Chemistry, 2016, 94, 1144-1150.	0.6	21
45	Pentlandite rocks as sustainable and stable efficient electrocatalysts for hydrogen generation. Nature Communications, 2016, 7, 12269.	5.8	150
46	Model Study of Thermoresponsive Behavior of Metalâ€“Organic Frameworks Modulated by Linker Functionalization. Journal of Physical Chemistry C, 2016, 120, 6835-6841.	1.5	14
47	Coarse graining of force fields for metalâ€“organic frameworks. Dalton Transactions, 2016, 45, 4370-4379.	1.6	32
48	Isoreticular isomerism in 4,4-connected paddle-wheel metalâ€“organic frameworks: structural prediction by the reverse topological approach. CrystEngComm, 2015, 17, 344-352.	1.3	30
49	QuickFF: A program for a quick and easy derivation of force fields for metalâ€organic frameworks from ab initio input. Journal of Computational Chemistry, 2015, 36, 1015-1027.	1.5	132
50	Rotational and translational dynamics of CO2 adsorbed in MOF Zn2(bdc)2(dabco). Microporous and Mesoporous Materials, 2015, 216, 75-81.	2.2	20
51	Almost Enclosed Buckyball Joints: Synthesis, Complex Formation, and Computational Simulations of Pentypticeneâ€Extended Tribenzotriquinacene. ChemPhysChem, 2014, 15, 3855-3863.	1.0	21
52	Ferrocene in the metalâ€“organic framework MOF-5 studied by homo- and heteronuclear correlation NMR and MD simulation. Microporous and Mesoporous Materials, 2014, 186, 130-136.	2.2	5
53	Surface Termination of the Metal-Organic Framework HKUST-1: A Theoretical Investigation. Journal of Physical Chemistry Letters, 2014, 5, 3206-3210.	2.1	65
54	Tribenzotriquinacene Receptors for C₆₀â€...Fullerene Rotors: Towards C₃ Symmetrical Chiral Stators for Unidirectionally Operating Nanoratchets. Chemistry - A European Journal, 2014, 20, 9100-9110.	1.7	30

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55	Structural Complexity in Metalâ€“Organic Frameworks: Simultaneous Modification of Open Metal Sites and Hierarchical Porosity by Systematic Doping with Defective Linkers. Journal of the American Chemical Society, 2014, 136, 9627-9636.	6.6	240
56	A Cryogenically Flexible Covalent Organic Framework for Efficient Hydrogen Isotope Separation by Quantum Sieving. Angewandte Chemie - International Edition, 2013, 52, 13219-13222.	7.2	183
57	Hypothetical 3D-periodic covalent organic frameworks: exploring the possibilities by a first principles derived force field. CrystEngComm, 2013, 15, 1551.	1.3	57
58	CO Adsorption on a Mixed-Valence Ruthenium Metalâ€“Organic Framework Studied by UHV-FTIR Spectroscopy and DFT Calculations. Journal of Physical Chemistry C, 2013, 117, 5658-5666.	1.5	48
59	MOFâ€FF â€“ A flexible firstâ€principles derived force field for metalâ€organic frameworks. Physica Status Solidi (B): Basic Research, 2013, 250, 1128-1141.	0.7	162
60	Prediction of Structure and Properties of Boron-Based Covalent Organic Frameworks by a First-Principles Derived Force Field. Journal of Physical Chemistry C, 2012, 116, 4921-4929.	1.5	52
61	Advanced buckyball joints: synthesis, complex formation and computational simulations of centrohexaindane-extended tribenzotriquinacene receptors for C60 fullerene. Dalton Transactions, 2012, 41, 5995.	1.6	36
62	Adsorption of Hydrocarbons in Metalâ€“Organic Frameworks: A Force Field Benchmark on the Example of Benzene in Metalâ€“Organic Framework 5. Journal of Physical Chemistry C, 2012, 116, 15369-15377.	1.5	14
63	Orbital directing effects in copper and zinc based paddle-wheel metal organic frameworks: the origin of flexibility. Journal of Materials Chemistry, 2012, 22, 10249.	6.7	56
64	Lowâ€Temperature CO Oxidation over Cuâ€Based Metalâ€“Organic Frameworks Monitored by using FTIR Spectroscopy. ChemCatChem, 2012, 4, 755-759.	1.8	38
65	Exploring Network Topologies of Copper Paddle Wheel Based Metalâ€“Organic Frameworks with a First-Principles Derived Force Field. Journal of Physical Chemistry C, 2011, 115, 15133-15139.	1.5	47
66	NMR studies of benzene mobility in metal-organic framework MOF-5. EPJ Applied Physics, 2011, 55, 20702.	0.3	11
67	OberflÃchenchemie Metallâ€organischer GerÃ¼ste an der FlÃ¼ssigâ€festâ€Grenzfläche. Angewandte Chemie, 2011, 123, 184-208.	1.6	43
68	Surface Chemistry of Metalâ€“Organic Frameworks at the Liquidâ€“Solid Interface. Angewandte Chemie - International Edition, 2011, 50, 176-199.	7.2	292
69	Flexibility and Sorption Selectivity in Rigid Metalâ€“Organic Frameworks: The Impact of Etherâ€Functionalised Linkers. Chemistry - A European Journal, 2010, 16, 14296-14306.	1.7	128
70	Atomistic theoretical models for nanoporous hybrid materials. Microporous and Mesoporous Materials, 2010, 129, 304-318.	2.2	46
71	A novel method to measure diffusion coefficients in porous metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2010, 12, 8092.	1.3	141
72	First-Principles-Derived Force Field for Copper Paddle-Wheel-Based Metalâ”Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 14402-14409.	1.5	85

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73	Substituentâ€Free Gallium by Hydrogenolysis of Coordinated GaCp*: Synthesis and Structure of Highly Fluxional [Ru₂(Ga)(GaCp*)₇(H)₃]. Angewandte Chemie - International Edition, 2009, 48, 3872-3876.	7.2	42
74	Cover Picture: Substituent-Free Gallium by Hydrogenolysis of Coordinated GaCp*: Synthesis and Structure of Highly Fluxional [Ru2(Ga)(GaCp*)7(H)3] (Angew. Chem. Int. Ed. 21/2009). Angewandte Chemie - International Edition, 2009, 48, 3713-3713.	7.2	0
75	Mechanism of benzene diffusion in MOF-5: A molecular dynamics investigation. Microporous and Mesoporous Materials, 2009, 125, 90-96.	2.2	45
76	Systematic First Principles Parameterization of Force Fields for Metalâ^'Organic Frameworks using a Genetic Algorithm Approach. Journal of Physical Chemistry B, 2009, 113, 1341-1352.	1.2	102
77	A Consistent Force Field for the Carboxylate Group. Journal of Chemical Theory and Computation, 2009, 5, 2822-2834.	2.3	21
78	A parallel multigrid accelerated Poisson solver for ab initio molecular dynamics applications. Computing and Visualization in Science, 2008, 11, 115-122.	1.2	11
79	An Accurate Force Field Model for the Strain Energy Analysis of the Covalent Organic Framework COF-102. Journal of the American Chemical Society, 2008, 130, 12600-12601.	6.6	56
80	Conformational Isomerism in the Isoreticular Metal Organic Framework Family: A Force Field Investigation. Journal of Physical Chemistry C, 2008, 112, 14980-14987.	1.5	50
81	Molecular Dynamics Simulation of Benzene Diffusion in MOF-5: Importance of Lattice Dynamics. Angewandte Chemie - International Edition, 2007, 46, 463-466.	7.2	195
82	Ab initio parametrized MM3 force field for the metal-organic framework MOF-5. Journal of Computational Chemistry, 2007, 28, 1169-1176.	1.5	112
83	Thermodynamic Stability of Small GanNn Clusters as Intermediates in GaN CVD. Chemical Vapor Deposition, 2007, 13, 84-90.	1.4	6
84	Theoretical determination of accurate rate constants: Application to the decomposition of a single-molecule precursor. Surface and Coatings Technology, 2007, 201, 8818-8824.	2.2	2
85	Carâ€"Parrinello molecular dynamics using real space wavefunctions. Physica Status Solidi (B): Basic Research, 2006, 243, 1001-1015.	0.7	15
86	Loading of porous metalâ€"organic open frameworks with organometallic CVD precursors: inclusion compounds of the type [LnM]a@MOF-5. Journal of Materials Chemistry, 2006, 16, 2464-2472.	6.7	204
87	The [Ga2(C5Me5)]+ Ion: Bipyramidal Double-Cone Structure and Weakly Coordinated, Monovalent Ga+. Angewandte Chemie - International Edition, 2006, 45, 1074-1076.	7.2	64
88	The [Ga2(C5Me5)]+ Ion: Bipyramidal Double-Cone Structure and Weakly Coordinated, Monovalent Ga+. Angewandte Chemie - International Edition, 2006, 45, 1674-1674.	7.2	12
89	A general and efficient pseudopotential Fourier filtering scheme for real space methods using mask functions. Journal of Chemical Physics, 2006, 124, 174102.	1.2	32
90	Calculation of rotational partition functions by an efficient Monte Carlo importance sampling technique. Journal of Computational Chemistry, 2005, 26, 1579-1591.	1.5	13

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91	A Multiscale Simulation Approach for the MOCVD of GaN Using a Single-Molecule Precursor in a Vertical Stagnation Flow Reactor. Chemical Vapor Deposition, 2005, 11, 306-316.	1.4	9
92	Metal@MOF: Loading of Highly Porous Coordination Polymers Host Lattices by Metal Organic Chemical Vapor Deposition. Angewandte Chemie - International Edition, 2005, 44, 6237-6241.	7.2	662
93	Gas Phase Chemistry in Gallium Nitride CVD:Â Theoretical Determination of the Arrhenius Parameters for the First Gaâ^'C Bond Homolysis of Trimethylgallium. Journal of Physical Chemistry A, 2005, 109, 2623-2630.	1.1	25
94	Cycloheptatrienylâ^'Cyclopentadienylâ^'Zirconium Sandwich Complexes:Â Structure and Bondingâ€. Organometallics, 2005, 24, 3163-3171.	1.1	50
95	Mechanistic Insights into an Unprecedented Câ^'C Bond Activation on a Rh/Ga Bimetallic Complex:Â A Combined Experimental/Computational Approach. Journal of the American Chemical Society, 2005, 127, 17068-17078.	6.6	58
96	Car-Parrinello simulations with a real space method. Journal of Computational Chemistry, 2004, 25, 799-812.	1.5	24
97	The reaction of RhCp*(CH3)2(L) (L = pyridine, dmso) with GaCp* and AlCp*: A new type of carbonâ€“carbon bond activation reaction. Dalton Transactions, 2004, , 3171-3172.	1.6	27
98	Theoretical Investigation of the Gas-Phase Decomposition of Ga(N3)2Et as a Model for a Single-Molecule GaN Precursor. Chemical Vapor Deposition, 2003, 9, 272-278.	1.4	11
99	Ab initio molecular dynamics with a continuum solvation model. Journal of Chemical Physics, 2003, 118, 1089-1100.	1.2	38
100	Diiminates and Diamides as Ligands in Polymerization Catalysts with M(III) (M = Ti, V, Cr) Metal Centers. A Theoretical Study. Organometallics, 2000, 19, 3069-3076.	1.1	25
101	Density Functional Study of the Migratory Insertion Step in the Carbonylation of Methanol Catalyzed by [M(CO)2I2]-(M = Rh, Ir). Organometallics, 2000, 19, 1973-1982.	1.1	62
102	Polymerization Catalysts with dnElectrons (n= 1â^'4):Â A Theoretical Study. Organometallics, 2000, 19, 2756-2765.	1.1	41
103	Ethylene-polymerization by surface supported Cr(IV) species: possible reaction mechanisms revisited by theoretical calculations. Canadian Journal of Chemistry, 2000, 78, 265-269.	0.6	35
104	A Combined QM/MM Method for the Determination of Regioselectivities in Rhodium-Catalyzed Hydroformylation. Organometallics, 1998, 17, 4828-4834.	1.1	56
105	A Molecular Model To Explain and Predict the Stereoselectivity in Rhodium-Catalyzed Hydroformylationâ€. Organometallics, 1998, 17, 2141-2143.	1.1	70
106	Coordination Chemistry and Mechanisms of Metal-Catalyzed CC-Coupling Reactions. 10.â€Ligand Dissociation in Rhodium-Catalyzed Hydroformylation:Â A Theoretical Studyâ€¡. Organometallics, 1997, 16, 701-708.	1.1	77
107	Feâ^'B Bonding in (Dibromoboryl)ferrocene:Â A Structural and Theoretical Investigation. Organometallics, 1996, 15, 1188-1194.	1.1	90
108	Structure and Metal Coordination of the Diphosphine 2,2'-Bis((diphenylphosphino)methyl)-1,1'-binaphthyl (NAPHOS). Organometallics, 1995, 14, 1961-1968.	1.1	43

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109	Materials Chemistry of Group 13 Nitrides. , 0, , 49-80.		14