Michael Fischer

List of Publications by Year
in descending order

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71 papers	1,553 citations	257357 24 h-index	330025 37 g-index
103 all docs	103 docs citations	103 times ranked	1883 citing authors

#	Article	IF	Citations
1	Aluminum to germanium inversion in mulliteâ€type RAlGeO₅: Characterization of a rare phenomenon for RÂ=ÂY, Smâ€“Lu. Journal of the American Ceramic Society, 2022, 105, 728-741.	1.9	4
2	Crystal Structures of Two Titanium Phosphate-Based Proton Conductors: Ab Initio Structure Solution and Materials Properties. Inorganic Chemistry, 2022, 61, 2379-2390.	1.9	7
3	Elucidating the Germanium Distribution in ITQâ€13 Zeolites by Density Functional Theory**. Chemistry - A European Journal, 2022, 28, .	1.7	3
4	Local Distortions in a Prototypical Zeolite Framework Containing Double Fourâ€Ring Cages: The Role of Framework Composition and Organic Guests**. ChemPhysChem, 2021, 22, 40-54.	1.0	5
5	Advanced characterisation techniques: multi-scale, in situ, and time-resolved: general discussion. Faraday Discussions, 2021, 225, 152-167.	1.6	2
6	Polymorphism of dimethylaminoborane N(CH₃)₂-BH₂. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 299-306.	0.5	1
7	Fluoride Anions in All-Silica Zeolites: Studying Preferred Fluoride Sites and Dynamic Disorder with Density Functional Theory Calculations. Journal of Physical Chemistry C, 2021, 125, 8825-8839.	1.5	10
8	Phonons and Adsorption-Induced Deformations in ZIFs: Is It Really a Gate Opening?. Journal of Physical Chemistry C, 2021, 125, 7999-8005.	1.5	10
9	What Is Being Measured with P-Bearing NMR Probe Molecules Adsorbed on Zeolites?. Journal of the American Chemical Society, 2021, 143, 13616-13623.	6.6	27
10	Revisiting the Structure of Calcined and Hydrated AlPOâ€11 with DFTâ€Based Molecular Dynamics Simulations**. ChemPhysChem, 2021, 22, 2063-2077.	1.0	8
11	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
12	Effect of low frequency phonons on structural properties of ZIFs with SOD topology. Microporous and Mesoporous Materials, 2020, 304, 109132.	2.2	13
13	A computational study of the interaction of C2 hydrocarbons with CuBTC. Computational Materials Science, 2020, 173, 109438.	1.4	5
14	KLi₂RE(BO₃)₂ (RE = Dy, Ho, Er, Tm, Yb, and Y): Structural, Spectroscopic, And Thermogravimetric Studies on a Series of Mixed-Alkali Rare-Earth Orthoborates. Inorganic Chemistry, 2020, 59, 18214-18224.	1.9	5
15	Influence of Organic Structure-Directing Agents on Fluoride Dynamics in As-Synthesized Silicalite-1. Journal of Physical Chemistry C, 2020, 124, 5690-5701.	1.5	11
16	Simulation-based evaluation of zeolite adsorbents for the removal of emerging contaminants. Materials Advances, 2020, 1, 86-98.	2.6	17
17	The modulated low-temperature structure of malayaite, CaSnOSiO₄. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 316-321.	0.5	1
18	Modelling crystalline microporous materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 419-420.	0.4	0

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19	Proton Acidity and Proton Mobility in ECRâ€40, a Silicoaluminophosphate that Violates LÃ¶wenstein's Rule. Chemistry - A European Journal, 2019, 25, 13579-13590.	1.7	6
20	Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO2 and AlPO4 frameworks. Journal of Chemical Physics, 2019, 150, 094102.	1.2	24
21	First-Principles Study of AlPO4-H3, a Hydrated Aluminophosphate Zeotype Containing Two Different Types of Adsorbed Water Molecules. Molecules, 2019, 24, 922.	1.7	9
22	Local Environment and Dynamic Behavior of Fluoride Anions in Silicogermanate Zeolites: A Computational Study of the AST Framework. Journal of Physical Chemistry C, 2019, 123, 1852-1865.	1.5	12
23	Template effects on the pressure-dependent behavior of chabazite-type fluoroaluminophosphates: a computational approach. Physics and Chemistry of Minerals, 2019, 46, 385-401.	0.3	10
24	Low-temperature anharmonicity and symmetry breaking in the sodalite |Na8I2|[AlSiO4]6. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 219-228.	0.4	2
25	A Multifaceted Study of Methane Adsorption in Metalâ€“Organic Frameworks by Using Three Complementary Techniques. Chemistry - A European Journal, 2018, 24, 7866-7881.	1.7	29
26	Thermal properties of 2:1 bismuth borate: Temperatureâ€dependent characterizations of lone electron pairs. Journal of the American Ceramic Society, 2018, 102, 2154.	1.9	2
27	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. Journal of Chemical Physics, 2018, 149, 064110.	1.2	23
28	Porous aluminophosphates as adsorbents for the separation of CO₂/CH₄and CH₄/N₂mixtures â€“ a Monte Carlo simulation study. Sustainable Energy and Fuels, 2018, 2, 1749-1763.	2.5	14
29	Frontispiece: A Multifaceted Study of Methane Adsorption in Metal-Organic Frameworks by Using Three Complementary Techniques. Chemistry - A European Journal, 2018, 24, .	1.7	0
30	New Model for Predicting Adsorption of Polar Molecules in Metalâ€“Organic Frameworks with Unsaturated Metal Sites. Journal of Physical Chemistry Letters, 2018, 9, 3544-3553.	2.1	29
31	Phase transitions of titanite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaTiSiO</mml:mi><mml:mn>5</mml:mn></mml:msub from density functional perturbation theory. Physical Review Materials, 2018, 2, .	0.9	6
32	Accurate structures and energetics of neutral-framework zeotypes from dispersion-corrected DFT calculations. Journal of Chemical Physics, 2017, 146, 174111.	1.2	30
33	A Transferable Model for Adsorption in MOFs with Unsaturated Metal Sites. Journal of Physical Chemistry C, 2017, 121, 441-458.	1.5	28
34	Crystal chemical characterization of mullite-type aluminum borate compounds. Journal of Solid State Chemistry, 2017, 247, 173-187.	1.4	16
35	â€œExplosiveâ€•synthesis of metal-formate frameworks for methane capture: an experimental and computational study. Chemical Communications, 2017, 53, 11437-11440.	2.2	25
36	Thermal behavior of mullite between 4 K and 1320 K. Journal of the American Ceramic Society, 2017, 100, 5259-5273.	1.9	14

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37	Computational evaluation of aluminophosphate zeotypes for CO₂/N₂separation. Physical Chemistry Chemical Physics, 2017, 19, 22801-22812.	1.3	13
38	Molecular structure of diethylaminoalane in the solid state: an X-ray powder diffraction, DFT calculation and Raman spectroscopy study. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 232-240.	0.5	6
39	Thermal expansion modeling of framework-type Na[AsW 2 O 9] and K[AsW 2 O 9]. Materials Research Bulletin, 2016, 84, 273-282.	2.7	11
40	Benchmarking DFT-GGA calculations for the structure optimisation of neutral-framework zeotypes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	38
41	Interaction of water with (silico)aluminophosphate zeotypes: a comparative investigation using dispersion-corrected DFT. Physical Chemistry Chemical Physics, 2016, 18, 15738-15750.	1.3	29
42	DFT-based evaluation of porous metal formates for the storage and separation of small molecules. Microporous and Mesoporous Materials, 2016, 219, 249-257.	2.2	11
43	A DFT-D study of the interaction of methane, carbon monoxide, and nitrogen with cation-exchanged SAPO-34. Zeitschrift Fur Kristallographie - Crystalline Materials, 2015, 230, 311-323.	0.4	2
44	Structure and bonding of water molecules in zeolite hosts: Benchmarking plane-wave DFT against crystal structure data. Zeitschrift Fur Kristallographie - Crystalline Materials, 2015, 230, 325-336.	0.4	33
45	Thermal expansion of mullite-type Bi2Al4O9: A study by X-ray diffraction, vibrational spectroscopy and density functional theory. Journal of Solid State Chemistry, 2015, 229, 87-96.	1.4	29
46	CO adsorption complexes in zeolites: How does the inclusion of dispersion interactions affect predictions made from DFT calculations? The case of Na-CHA. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	17
47	Water adsorption in SAPO-34: elucidating the role of local heterogeneities and defects using dispersion-corrected DFT calculations. Physical Chemistry Chemical Physics, 2015, 17, 25260-25271.	1.3	30
48	Modeling the Adsorption of Small Molecules at Coordinatively Unsaturated Metal Sites: Density Functional Theory and Molecular Mechanics Approaches. , 2015, , 113-174.		0
49	Computational approaches to study adsorption in MOFs with unsaturated metal sites. Molecular Simulation, 2014, 40, 537-556.	0.9	75
50	Cation-exchanged SAPO-34 for adsorption-based hydrocarbon separations: predictions from dispersion-corrected DFT calculations. Physical Chemistry Chemical Physics, 2014, 16, 21062-21072.	1.3	14
51	Porous M^{II}/Pyrimidineâ€4,6â€Dicarboxylato Neutral Frameworks: Synthetic Influence on the Adsorption Capacity and Evaluation of CO₂â€Adsorbent Interactions. Chemistry - A European Journal, 2014, 20, 1554-1568.	1.7	22
52	Interaction of hydrogen and carbon dioxide with sod-type zeolitic imidazolate frameworks: a periodic DFT-D study. CrystEngComm, 2014, 16, 1934.	1.3	44
53	Accurate Model for Predicting Adsorption of Olefins and Paraffins on MOFs with Open Metal Sites. Industrial & Engineering Chemistry Research, 2014, 53, 15475-15487.	1.8	52
54	Water adsorption on a copper formate paddlewheel model of CuBTC: A comparative MP2 and DFT study. Chemical Physics Letters, 2013, 587, 7-13.	1.2	40

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55	Modeling CO₂ Adsorption in Zeolites Using DFT-Derived Charges: Comparing System-Specific and Generic Models. Journal of Physical Chemistry C, 2013, 117, 24446-24454.	1.5	21
56	A dispersion-corrected density-functional theory study of small molecules adsorbed in alkali-exchanged chabazites. Zeitschrift Fur Kristallographie - Crystalline Materials, 2013, 228, 124-133.	0.4	13
57	Identifying Promising Zeolite Frameworks for Separation Applications: A Building-Block-Based Approach. Journal of Physical Chemistry C, 2013, 117, 17099-17110.	1.5	19
58	Gas Adsorption Properties and Selectivity in CuII/Adeninato/Carboxylato Metal-Biomolecule Frameworks. European Journal of Inorganic Chemistry, 2012, 2012, 5921-5933.	1.0	31
59	Influence of Zeolite Topology on CO₂/N₂ Separation Behavior: Force-Field Simulations Using a DFT-Derived Charge Model. Journal of Physical Chemistry C, 2012, 116, 26449-26463.	1.5	51
60	Modeling Adsorption in Metalâ€“Organic Frameworks with Open Metal Sites: Propane/Propylene Separations. Langmuir, 2012, 28, 8537-8549.	1.6	70
61	Metalâ€“organic frameworks and related materials for hydrogen purification: Interplay of pore size and pore wall polarity. RSC Advances, 2012, 2, 4382.	1.7	37
62	A new series of isoreticular copper-based metalâ€“organic frameworks containing non-linear linkers with different group 14 central atoms. Journal of Materials Chemistry, 2012, 22, 10294.	6.7	9
63	An Interpenetrated Metalâ€“Organic Framework and Its Gas Storage Behavior: Simulation and Experiment. Inorganic Chemistry, 2011, 50, 11055-11063.	1.9	43
64	New Microporous Materials for Acetylene Storage and C₂H₂/CO₂ Separation: Insights from Molecular Simulations. ChemPhysChem, 2010, 11, 2220-2229.	1.0	118
65	Molecular simulation of hydrogen adsorption in metal-organic frameworks. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2010, 357, 35-42.	2.3	33
66	Kleine Poren â€” groÃŸe Wirkung. Nachrichten Aus Der Chemie, 2010, 58, 1003-1007.	0.0	3
67	Accurate Prediction of Hydrogen Adsorption in Metalâˆ’Organic Frameworks with Unsaturated Metal Sites via a Combined Density-Functional Theory and Molecular Mechanics Approach. Journal of Physical Chemistry C, 2010, 114, 19116-19126.	1.5	46
68	Preferred Hydrogen Adsorption Sites in Various MOFsâ€”A Comparative Computational Study. ChemPhysChem, 2009, 10, 2647-2657.	1.0	75
69	Highly Porous Metal-Organic Framework Containing a Novel Organosilicon Linker âˆ’ A Promising Material for Hydrogen Storage. Inorganic Chemistry, 2009, 48, 6559-6565.	1.9	60
70	Gas Storage in Porous Solids. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2007-2007.	0.6	1
71	Structure and stability ofCd2Nb2O7andCd2Ta2O7explored byab initiocalculations. Physical Review B, 2008, 78, .	1.1	43