

Michael Fischer

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/63702/publications.pdf>

Version: 2024-02-01

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	New Microporous Materials for Acetylene Storage and C ₂ H ₂ /CO ₂ Separation: Insights from Molecular Simulations. ChemPhysChem, 2010, 11, 2220-2229.	1.0	118
2	Preferred Hydrogen Adsorption Sites in Various MOFs—A Comparative Computational Study. ChemPhysChem, 2009, 10, 2647-2657.	1.0	75
3	Computational approaches to study adsorption in MOFs with unsaturated metal sites. Molecular Simulation, 2014, 40, 537-556.	0.9	75
4	Modeling Adsorption in Metal-Organic Frameworks with Open Metal Sites: Propane/Propylene Separations. Langmuir, 2012, 28, 8537-8549.	1.6	70
5	Highly Porous Metal-Organic Framework Containing a Novel Organosilicon Linker — A Promising Material for Hydrogen Storage. Inorganic Chemistry, 2009, 48, 6559-6565.	1.9	60
6	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
7	Influence of Zeolite Topology on CO ₂ /N ₂ Separation Behavior: Force-Field Simulations Using a DFT-Derived Charge Model. Journal of Physical Chemistry C, 2012, 116, 26449-26463.	1.5	51
8	Accurate Prediction of Hydrogen Adsorption in Metal-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
9	Interaction of hydrogen and carbon dioxide with sod-type zeolitic imidazolate frameworks: a periodic DFT-D study. CrystEngComm, 2014, 16, 1934.	1.3	44
10	Structure and stability of Cd ₂ Nb ₂ O ₇ and Cd ₂ Ta ₂ O ₇ explored by ab initio calculations. Physical Review B, 2008, 78, .	1.1	43
11	An Interpenetrated Metal-Organic Framework and Its Gas Storage Behavior: Simulation and Experiment. Inorganic Chemistry, 2011, 50, 11055-11063.	1.9	43
12	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
13	Benchmarking DFT-GGA calculations for the structure optimisation of neutral-framework zeotypes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	38
14	Metal-organic frameworks and related materials for hydrogen purification: Interplay of pore size and pore wall polarity. RSC Advances, 2012, 2, 4382.	1.7	37
15	Molecular simulation of hydrogen adsorption in metal-organic frameworks. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2010, 357, 35-42.	2.3	33
16	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
17	Gas Adsorption Properties and Selectivity in CuII/Adeninato/Carboxylato Metal-Biomolecule Frameworks. European Journal of Inorganic Chemistry, 2012, 2012, 5921-5933.	1.0	31
18	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

#	ARTICLE	IF	CITATIONS
19	Accurate structures and energetics of neutral-framework zeotypes from dispersion-corrected DFT calculations. <i>Journal of Chemical Physics</i> , 2017, 146, 174111.	1.2	30
20	Thermal expansion of mullite-type Bi ₂ Al ₄ O ₉ : A study by X-ray diffraction, vibrational spectroscopy and density functional theory. <i>Journal of Solid State Chemistry</i> , 2015, 229, 87-96.	1.4	29
21	Interaction of water with (silico)aluminophosphate zeotypes: a comparative investigation using dispersion-corrected DFT. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15738-15750.	1.3	29
22	A Multifaceted Study of Methane Adsorption in Metal-Organic Frameworks by Using Three Complementary Techniques. <i>Chemistry - A European Journal</i> , 2018, 24, 7866-7881.	1.7	29
23	New Model for Predicting Adsorption of Polar Molecules in Metal-Organic Frameworks with Unsaturated Metal Sites. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3544-3553.	2.1	29
24	A Transferable Model for Adsorption in MOFs with Unsaturated Metal Sites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 441-458.	1.5	28
25	What Is Being Measured with P-Bearing NMR Probe Molecules Adsorbed on Zeolites?. <i>Journal of the American Chemical Society</i> , 2021, 143, 13616-13623.	6.6	27
26	Explosive-synthesis of metal-formate frameworks for methane capture: an experimental and computational study. <i>Chemical Communications</i> , 2017, 53, 11437-11440.	2.2	25
27	Benchmarking the performance of approximate van der Waals methods for the structural and energetic properties of SiO ₂ and AlPO ₄ frameworks. <i>Journal of Chemical Physics</i> , 2019, 150, 094102.	1.2	24
28	Benchmarking of GGA density functionals for modeling structures of nanoporous, rigid and flexible MOFs. <i>Journal of Chemical Physics</i> , 2018, 149, 064110.	1.2	23
29	Porous M ^{II} /Pyrimidine-4,6-Dicarboxylato Neutral Frameworks: Synthetic Influence on the Adsorption Capacity and Evaluation of CO ₂ Adsorbent Interactions. <i>Chemistry - A European Journal</i> , 2014, 20, 1554-1568.	1.7	22
30	Modeling CO ₂ Adsorption in Zeolites Using DFT-Derived Charges: Comparing System-Specific and Generic Models. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24446-24454.	1.5	21
31	Identifying Promising Zeolite Frameworks for Separation Applications: A Building-Block-Based Approach. <i>Journal of Physical Chemistry C</i> , 2013, 117, 17099-17110.	1.5	19
32	CO adsorption complexes in zeolites: How does the inclusion of dispersion interactions affect predictions made from DFT calculations? The case of Na-CHA. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	17
33	Simulation-based evaluation of zeolite adsorbents for the removal of emerging contaminants. <i>Materials Advances</i> , 2020, 1, 86-98.	2.6	17
34	Crystal chemical characterization of mullite-type aluminum borate compounds. <i>Journal of Solid State Chemistry</i> , 2017, 247, 173-187.	1.4	16
35	Cation-exchanged SAPO-34 for adsorption-based hydrocarbon separations: predictions from dispersion-corrected DFT calculations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 21062-21072.	1.3	14
36	Thermal behavior of mullite between 4 K and 1320 K. <i>Journal of the American Ceramic Society</i> , 2017, 100, 5259-5273.	1.9	14

#	ARTICLE	IF	CITATIONS
37	Porous aluminophosphates as adsorbents for the separation of CO ₂ /CH ₄ and CH ₄ /N ₂ mixtures – a Monte Carlo simulation study. Sustainable Energy and Fuels, 2018, 2, 1749-1763.	2.5	14
38	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
39	Computational evaluation of aluminophosphate zeotypes for CO ₂ /N ₂ separation. Physical Chemistry Chemical Physics, 2017, 19, 22801-22812.	1.3	13
40	Effect of low frequency phonons on structural properties of ZIFs with SOD topology. Microporous and Mesoporous Materials, 2020, 304, 109132.	2.2	13
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	A new series of isorecticular copper-based metal-organic frameworks containing non-linear linkers with different group 14 central atoms. Journal of Materials Chemistry, 2012, 22, 10294.	6.7	9
49	First-Principles Study of AlPO ₄ -H ₃ , a Hydrated Aluminophosphate Zeotype Containing Two Different Types of Adsorbed Water Molecules. Molecules, 2019, 24, 922.	1.7	9
50	Revisiting the Structure of Calcined and Hydrated AlPO ₄ -11 with DFT-Based Molecular Dynamics Simulations**. ChemPhysChem, 2021, 22, 2063-2077.	1.0	8
51	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
52	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
53	Proton Acidity and Proton Mobility in ECR-40, a Silicoaluminophosphate that Violates L�wenzel's Rule. Chemistry - A European Journal, 2019, 25, 13579-13590.	1.7	6
54	Phase transitions of titanite CaTiSiO_5 from density functional perturbation theory. Physical Review Materials, 2018, 2, .	0.1	6

#	ARTICLE	IF	CITATIONS
55	A computational study of the interaction of C2 hydrocarbons with CuBTC. Computational Materials Science, 2020, 173, 109438.	1.4	5
56	$\text{KLi}_2\text{RE}(\text{BO}_3)_2$ (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
57	Local Distortions in a Prototypical Zeolite Framework Containing Double Four-Ring Cages: The Role of Framework Composition and Organic Guests**. ChemPhysChem, 2021, 22, 40-54.	1.0	5
58	Aluminum to germanium inversion in mullite-type AlGeO_5 : Characterization of a rare phenomenon for $\text{R}=\text{Y}, \text{Sm}-\text{Lu}$. Journal of the American Ceramic Society, 2022, 105, 728-741.	1.9	4
59	Kleine Poren – große Wirkung. Nachrichten Aus Der Chemie, 2010, 58, 1003-1007.	0.0	3
60	Elucidating the Germanium Distribution in ITQ-13 Zeolites by Density Functional Theory**. Chemistry - A European Journal, 2022, 28, .	1.7	3
61	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
62	Thermal properties of 2:1 bismuth borate: Temperature-dependent characterizations of lone electron pairs. Journal of the American Ceramic Society, 2018, 102, 2154.	1.9	2
63	Low-temperature anharmonicity and symmetry breaking in the sodalite $ \text{Na}_8\text{I}_2 [\text{AlSiO}_4]_6$. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 219-228.	0.4	2
64	Advanced characterisation techniques: multi-scale, <i>in situ</i> , and time-resolved: general discussion. Faraday Discussions, 2021, 225, 152-167.	1.6	2
65	Gas Storage in Porous Solids. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2007-2007.	0.6	1
66	Polymorphism of dimethylaminoborane $\text{N}(\text{CH}_3)_2\text{-BH}_2$. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 299-306.	0.5	1
67	Novel computational tools: general discussion. Faraday Discussions, 2021, 225, 341-357.	1.6	1
68	The modulated low-temperature structure of malayaite, CaSnOSiO_4 . Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 316-321.	0.5	1
69	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
70	Modelling crystalline microporous materials. Zeitschrift Fur Kristallographie - Crystalline Materials, 2019, 234, 419-420.	0.4	0
71	Modeling the Adsorption of Small Molecules at Coordinatively Unsaturated Metal Sites: Density Functional Theory and Molecular Mechanics Approaches. , 2015, , 113-174.		0