Daniel W Siderius

List of Publications by Year
in descending order

47 papers	846 citations	566801 15 h-index	500791 28 g-index
51 all docs	51 docs citations	51 times ranked	955 citing authors

#	Article	IF	Citations
1	Data-Driven Matching of Experimental Crystal Structures and Gas Adsorption Isotherms of Metalâ€“Organic Frameworks. Journal of Chemical & Engineering Data, 2022, 67, 1743-1756.	1.0	6
2	Reference surface excess isotherms for carbon dioxide adsorption on ammonium ZSM-5 at various temperatures. Adsorption, 2022, 28, 15-25.	1.4	2
3	Comments on â€œMonte Carlo simulations for water adsorption in porous materials: Best practices and new insightsâ€• AIChE Journal, 2022, 68, .	1.8	1
4	Graph neural network predictions of metal organic framework CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e488" altimg="si38.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> adsorption properties. Computational Materials Science, 2022, 210, 111388.	1.4	19
5	Preface to Adsorption and Diffusion in Porous Materials Special Issue: Equilibrium Adsorption Data for Energy and Environmental Applications. Journal of Chemical & Engineering Data, 2022, 67, 1597-1598.	1.0	1
6	Synthesis, structural and sorption characterization of a Hofmann compound, Ni(3-methy-4,4â€²-bipyridine)[Ni(CN)4]. Polyhedron, 2021, 200, 115132.	1.0	5
7	Crystal structure, sorption properties, and electronic structure of flexible MOF, (Ni-4,4â€²azopyridine)[Ni(CN)4]. Solid State Sciences, 2021, 118, 106646.	1.5	5
8	Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials. Chemistry of Materials, 2021, 33, 7203-7216.	3.2	11
9	Digitization of Adsorption Isotherms from "The Thermodynamics and Hysteresis of Adsorption". Journal of Research of the National Institute of Standards and Technology, 2021, 126, .	0.4	1
10	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. Journal of Physical Chemistry C, 2020, 124, 16350-16361.	1.5	4
11	The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation. Molecular Simulation, 2019, 45, 1082-1121.	0.9	74
12	Powder X-ray structural studies and reference diffraction patterns for three forms of porous aluminum terephthalate, MIL-53(Al). Powder Diffraction, 2019, 34, 216-226.	0.4	4
13	Understanding Material Characteristics through Signature Traits from Helium Pycnometry. Langmuir, 2019, 35, 2115-2122.	1.6	30
14	Best Practices for Quantification of Uncertainty and Sampling Quality in Molecular Simulations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	93
15	Molecular simulation of capillary phase transitions in flexible porous materials. Journal of Chemical Physics, 2018, 148, 124115.	1.2	11
16	Synthesis and synchrotron X-ray characterization of two 2D Hoffman related compounds [Ni(p-Xylylenediamine)nNi(CN)4] and [Ni(p-tetrafluoroxylylenediamine)nNi(CN)4]. Solid State Sciences, 2018, 81, 12-18.	1.5	3
17	Electronic structure, pore size distribution, and sorption characterization of an unusual MOF, {[Ni(dpbz)][Ni(CN)4]}n, dpbz = 1,4-bis(4-pyridyl)benzene. Journal of Applied Physics, 2018, 123, 245105.	1.1	9
18	The ninth industrial fluid properties simulation challenge. Fluid Phase Equilibria, 2018, 476, 1-5.	1.4	7

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19	Relationship between pore-size distribution and flexibility of adsorbent materials: statistical mechanics and future material characterization techniques. Adsorption, 2017, 23, 593-602.	1.4	9
20	Connection Between Thermodynamics and Dynamics of Simple Fluids in Pores: Impact of Fluidâ€“Fluid Interaction Range and Fluidâ€“Solid Interaction Strength. Journal of Physical Chemistry C, 2017, 121, 16316-16327.	1.5	12
21	Quasi-Two-Dimensional Phase Transition of Methane Adsorbed in Cylindrical Silica Mesopores. Langmuir, 2017, 33, 14252-14262.	1.6	8
22	Position-Dependent Dynamics Explain Pore-Averaged Diffusion in Strongly Attractive Adsorptive Systems. Langmuir, 2017, 33, 13955-13963.	1.6	4
23	Modulusâ€“pressure equation for confined fluids. Journal of Chemical Physics, 2016, 145, 164505.	1.2	26
24	The Eighth Industrial Fluids Properties Simulation Challenge. Adsorption Science and Technology, 2016, 34, 3-12.	1.5	3
25	Adsorption, X-ray diffraction, photoelectron, and atomic emission spectroscopy benchmark studies for the eighth industrial fluid properties simulation challenge. Adsorption Science and Technology, 2016, 34, 13-41.	1.5	6
26	Relation between pore size and the compressibility of a confined fluid. Journal of Chemical Physics, 2015, 143, 194506.	1.2	38
27	Reference diffraction patterns, microstructure, and pore-size distribution for the copper (II) benzene-1,3,5-tricarboxylate metal organic framework (Cu-BTC) compounds. Powder Diffraction, 2015, 30, 2-13.	0.4	23
28	Elucidating the effects of adsorbent flexibility on fluid adsorption using simple models and flat-histogram sampling methods. Journal of Chemical Physics, 2014, 140, 244106.	1.2	27
29	Perfluorohexane adsorption in BCR-704 Faujasite zeolite benchmark studies for the seventh industrial fluid properties simulation challenge. Fluid Phase Equilibria, 2014, 366, 141-145.	1.4	4
30	The seventh industrial fluid properties simulation challenge. Fluid Phase Equilibria, 2014, 366, 136-140.	1.4	5
31	Connection between Thermodynamics and Dynamics of Simple Fluids in Highly Attractive Pores. Langmuir, 2013, 29, 14527-14535.	1.6	15
32	Use of the Grand Canonical Transition-Matrix Monte Carlo Method to Model Gas Adsorption in Porous Materials. Journal of Physical Chemistry C, 2013, 117, 5861-5872.	1.5	34
33	Improved synthesis and crystal structure of the flexible pillared layer porous coordination polymer: Ni(1,2-bis(4-pyridyl)ethylene)[Ni(CN)4]. CrystEngComm, 2013, 15, 4684.	1.3	22
34	Osmotic virial coefficients for model protein and colloidal solutions: Importance of ensemble constraints in the analysis of light scattering data. Journal of Chemical Physics, 2012, 136, 175102.	1.2	12
35	Time-Dependent CO₂ Sorption Hysteresis in a One-Dimensional Microporous Octahedral Molecular Sieve. Journal of the American Chemical Society, 2012, 134, 7944-7951.	6.6	74
36	Extension of scaled particle theory to inhomogeneous hard particle fluids. IV. Cavity growth at any distance relative to a planar hard wall. Physical Review E, 2011, 83, 031126.	0.8	1

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37	Extension of the Steele 10-4-3 potential for adsorption calculations in cylindrical, spherical, and other pore geometries. Journal of Chemical Physics, 2011, 135, 084703.	1.2	60
38	Thermodynamic and structural properties of finely discretized on-lattice hard-sphere fluids: Virial coefficients, free energies, and direct correlation functions. Journal of Chemical Physics, 2009, 131, 084503.	1.2	4
39	Predicting Gas Adsorption in Complex Microporous and Mesoporous Materials Using a New Density Functional Theory of Finely Discretized Lattice Fluids. Langmuir, 2009, 25, 1296-1299.	1.6	46
40	Structure, Thermodynamics, and Solubility in Tetromino Fluids. Langmuir, 2009, 25, 6702-6716.	1.6	32
41	On the Line Tension of Curved Boundary Layers. I. Boundary Thermodynamics. Journal of Physical Chemistry B, 2009, 113, 13849-13859.	1.2	4
42	On the generalized equipartition theorem in molecular dynamics ensembles and the microcanonical thermodynamics of small systems. Journal of Chemical Physics, 2008, 128, 124301.	1.2	32
43	Extension of scaled particle theory to inhomogeneous hard particle fluids. III. Entropic force exerted on a cavity that intersects a hard wall. Physical Review E, 2007, 75, 011108.	0.8	10
44	On the use of multiple interpolation functions in scaled particle theory to improve the predictions of the properties of the hard-sphere fluid. Journal of Chemical Physics, 2007, 127, 144502.	1.2	12
45	Thermodynamically Consistent Adaptation of Scaled Particle Theory to an Arbitrary Hard-Sphere Equation of State. Industrial & Engineering Chemistry Research, 2006, 45, 5489-5500.	1.8	16
46	Extension of scaled particle theory to inhomogeneous hard particle fluids. II. Theory and simulation of fluid structure surrounding a cavity that intersects a hard wall. Physical Review E, 2005, 71, 036142.	0.8	9
47	Extension of scaled particle theory to inhomogeneous hard particle fluids. I. Cavity growth at a hard wall. Physical Review E, 2005, 71, 036141.	0.8	12