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	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
2	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
3	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
4	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
5	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
6	Relation between pore size and the compressibility of a confined fluid. Journal of Chemical Physics, 2015, 143, 194506.	1.2	38
7	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
8	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
9	Structure, Thermodynamics, and Solubility in Tetromino Fluids. Langmuir, 2009, 25, 6702-6716.	1.6	32
10	Understanding Material Characteristics through Signature Traits from Helium Pycnometry. Langmuir, 2019, 35, 2115-2122.	1.6	30
11	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
12	Modulusâ€“pressure equation for confined fluids. Journal of Chemical Physics, 2016, 145, 164505.	1.2	26
13	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
14	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
15	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
16	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
17	Connection between Thermodynamics and Dynamics of Simple Fluids in Highly Attractive Pores. Langmuir, 2013, 29, 14527-14535.	1.6	15
18	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

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19	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
20	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
21	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
22	Molecular simulation of capillary phase transitions in flexible porous materials. Journal of Chemical Physics, 2018, 148, 124115.	1.2	11
23	Recommendation System to Predict Missing Adsorption Properties of Nanoporous Materials. Chemistry of Materials, 2021, 33, 7203-7216.	3.2	11
24	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
25	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
26	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
27	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
28	Quasi-Two-Dimensional Phase Transition of Methane Adsorbed in Cylindrical Silica Mesopores. Langmuir, 2017, 33, 14252-14262.	1.6	8
29	The ninth industrial fluid properties simulation challenge. Fluid Phase Equilibria, 2018, 476, 1-5.	1.4	7
30	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
31	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
32	The seventh industrial fluid properties simulation challenge. Fluid Phase Equilibria, 2014, 366, 136-140.	1.4	5
33	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
34	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
35	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
36	On the Line Tension of Curved Boundary Layers. I. Boundary Thermodynamics. Journal of Physical Chemistry B, 2009, 113, 13849-13859.	1.2	4

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37	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
38	Position-Dependent Dynamics Explain Pore-Averaged Diffusion in Strongly Attractive Adsorptive Systems. Langmuir, 2017, 33, 13955-13963.	1.6	4
39	Powder X-ray structural studies and reference diffraction patterns for three forms of porous aluminum terephthalate, MIL-53(A1). Powder Diffraction, 2019, 34, 216-226.	0.4	4
40	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. Journal of Physical Chemistry C, 2020, 124, 16350-16361.	1.5	4
41	The Eighth Industrial Fluids Properties Simulation Challenge. Adsorption Science and Technology, 2016, 34, 3-12.	1.5	3
42	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
43	Reference surface excess isotherms for carbon dioxide adsorption on ammonium ZSM-5 at various temperatures. Adsorption, 2022, 28, 15-25.	1.4	2
44	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
45	Comments on â€œMonte Carlo simulations for water adsorption in porous materials: Best practices and new insightsâ€• AIChE Journal, 2022, 68, .	1.8	1
46	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
47	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