

# Celine Merlet

## List of Publications by Year in descending order

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Version: 2024-02-01

40  
papers

4,411  
citations

257357

24  
h-index

289141

40  
g-index

41  
all docs

41  
docs citations

41  
times ranked

5295  
citing authors

#	ARTICLE	IF	CITATIONS
1	Elucidating Curvature-Capacitance Relationships in Carbon-Based Supercapacitors. <i>Physical Review Letters</i> , 2022, 128, 086001.	2.9	14
2	Probing and Interpreting the Porosity and Tortuosity Evolution of Li-O <sub>2</sub> Cathodes on Discharge through a Combined Experimental and Theoretical Approach. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4955-4967.	1.5	11
3	Simulations of Ionic Liquids Confined in Surface-Functionalized Nanoporous Carbons: Implications for Energy Storage. <i>ACS Applied Nano Materials</i> , 2021, 4, 4007-4015.	2.4	12
4	NMR studies of adsorption and diffusion in porous carbonaceous materials. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2021, 124-125, 57-84.	3.9	19
5	Mesoscopic simulations of the in situ NMR spectra of porous carbon based supercapacitors: electronic structure and adsorbent reorganisation effects. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15925-15934.	1.3	4
6	Carbonâ€“carbon supercapacitors: Beyond the average pore size or how electrolyte confinement and inaccessible pores affect the capacitance. <i>Journal of Chemical Physics</i> , 2021, 155, 184703.	1.2	17
7	Ionic Liquids under Confinement: From Systematic Variations of the Ion and Pore Sizes toward an Understanding of the Structure and Dynamics in Complex Porous Carbons. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 1789-1798.	4.0	39
8	Effects of functional groups and anion size on the charging mechanisms in layered electrode materials. <i>Energy Storage Materials</i> , 2020, 33, 460-469.	9.5	36
9	Computational Insights into Charge Storage Mechanisms of Supercapacitors. <i>Energy and Environmental Materials</i> , 2020, 3, 235-246.	7.3	49
10	Efficient prediction of nucleus independent chemical shifts for polycyclic aromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 13746-13755.	1.3	10
11	Local Distortions and Dynamics in Hydrated Y-Doped BaZrO <sub>3</sub> . <i>Journal of Physical Chemistry C</i> , 2020, 124, 16689-16701.	1.5	12
12	Text mining assisted review of the literature on Li-O <sub>2</sub> batteries. <i>JPhys Materials</i> , 2019, 2, 044004.	1.8	16
13	On the development of an original mesoscopic model to predict the capacitive properties of carbon-carbon supercapacitors. <i>Electrochimica Acta</i> , 2019, 327, 135022.	2.6	16
14	Carbons with Regular Pore Geometry Yield Fundamental Insights into Supercapacitor Charge Storage. <i>ACS Central Science</i> , 2019, 5, 1813-1823.	5.3	44
15	Stochasticity of Pores Interconnectivity in Liâ€“O <sub>2</sub> Batteries and its Impact on the Variations in Electrochemical Performance. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 791-797.	2.1	37
16	Structural Characterization of the Li-Ion Battery Cathode Materials LiTi <sub>x</sub> Mn <sub>2</sub> O <sub>4</sub> (0.2 ≤ x ≤ 1.5): A Combined Experimental & Li NMR and First-Principles Study. <i>Chemistry of Materials</i> , 2018, 30, 817-829.	3.2	27
17	Tracking Ionic Rearrangements and Interpreting Dynamic Volumetric Changes in Twoâ€“Dimensional Metal Carbide Supercapacitors: A Molecular Dynamics Simulation Study. <i>ChemSusChem</i> , 2018, 11, 1892-1899.	3.6	50
18	Importance of Incorporating Explicit 3D-Resolved Electrode Mesostructures in Liâ€“O <sub>2</sub> Battery Models. <i>ACS Applied Energy Materials</i> , 2018, 1, 6433-6441.	2.5	14

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19	Towards an atomistic understanding of disordered carbon electrode materials. <i>Chemical Communications</i> , 2018, 54, 5988-5991.	2.2	84
20	Tracking Ionic Rearrangements and Interpreting Dynamic Volumetric Changes in Two-Dimensional Metal Carbide Supercapacitors: A Molecular Dynamics Simulation Study. <i>ChemSusChem</i> , 2018, 11, 1889-1889.	3.6	3
21	Direct observation of ion dynamics in supercapacitor electrodes using in situ diffusion NMR spectroscopy. <i>Nature Energy</i> , 2017, 2, .	19.8	285
22	New Perspectives on the Charging Mechanisms of Supercapacitors. <i>Journal of the American Chemical Society</i> , 2016, 138, 5731-5744.	6.6	529
23	Molecular Dynamics Simulations of Electrochemical Energy Storage Devices. <i>Green Energy and Technology</i> , 2016, , 61-89.	0.4	3
24	Single Electrode Capacitances of Porous Carbons in Neat Ionic Liquid Electrolyte at 100°C: A Combined Experimental and Modeling Approach. <i>Journal of the Electrochemical Society</i> , 2015, 162, A5091-A5095.	1.3	32
25	Lattice simulation method to model diffusion and NMR spectra in porous materials. <i>Journal of Chemical Physics</i> , 2015, 142, 094701.	1.2	28
26	NMR Study of Ion Dynamics and Charge Storage in Ionic Liquid Supercapacitors. <i>Journal of the American Chemical Society</i> , 2015, 137, 7231-7242.	6.6	182
27	New Insights into the Structure of Nanoporous Carbons from NMR, Raman, and Pair Distribution Function Analysis. <i>Chemistry of Materials</i> , 2015, 27, 6848-6857.	3.2	88
28	On the Dynamics of Charging in Nanoporous Carbon-Based Supercapacitors. <i>ACS Nano</i> , 2014, 8, 1576-1583.	7.3	201
29	Carbon electrodes for energy storage: general discussion. <i>Faraday Discussions</i> , 2014, 172, 239-260.	1.6	11
30	The Electric Double Layer Has a Life of Its Own. <i>Journal of Physical Chemistry C</i> , 2014, 118, 18291-18298.	1.5	195
31	Computer simulations of ionic liquids at electrochemical interfaces. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15781.	1.3	148
32	Charge Fluctuations in Nanoscale Capacitors. <i>Physical Review Letters</i> , 2013, 111, 106102.	2.9	129
33	Highly confined ions store charge more efficiently in supercapacitors. <i>Nature Communications</i> , 2013, 4, 2701.	5.8	570
34	Simulating Supercapacitors: Can We Model Electrodes As Constant Charge Surfaces?. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 264-268.	2.1	220
35	Influence of solvation on the structural and capacitive properties of electrical double layer capacitors. <i>Electrochimica Acta</i> , 2013, 101, 262-271.	2.6	96
36	New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7687-7693.	1.5	126

#	ARTICLE	IF	CITATIONS
37	On the molecular origin of supercapacitance in nanoporous carbon electrodes. <i>Nature Materials</i> , 2012, 11, 306-310.	13.3	861
38	Imidazolium Ionic Liquid Interfaces with Vapor and Graphite: Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16613-16618.	1.5	139
39	Thermal conductivity of ionic systems from equilibrium molecular dynamics. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 102101.	0.7	30
40	Internal mobilities and diffusion in an ionic liquid mixture. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 14109.	1.3	24