Celine Merlet

List of Publications by Year in descending order

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40 papers	4,411 citations	257450 24 h-index	289244 40 g-index
41 all docs	41 docs citations	41 times ranked	5295 citing authors

#	Article	IF	Citations
1	On the molecular origin of supercapacitance in nanoporous carbon electrodes. Nature Materials, 2012, 11, 306-310.	27.5	861
2	Highly confined ions store charge more efficiently in supercapacitors. Nature Communications, 2013, 4, 2701.	12.8	570
3	New Perspectives on the Charging Mechanisms of Supercapacitors. Journal of the American Chemical Society, 2016, 138, 5731-5744.	13.7	529
4	Direct observation of ion dynamics in supercapacitor electrodes using inÂsitu diffusion NMR spectroscopy. Nature Energy, 2017, 2, .	39.5	285
5	Simulating Supercapacitors: Can We Model Electrodes As Constant Charge Surfaces?. Journal of Physical Chemistry Letters, 2013, 4, 264-268.	4.6	220
6	On the Dynamics of Charging in Nanoporous Carbon-Based Supercapacitors. ACS Nano, 2014, 8, 1576-1583.	14.6	201
7	The Electric Double Layer Has a Life of Its Own. Journal of Physical Chemistry C, 2014, 118, 18291-18298.	3.1	195
8	NMR Study of Ion Dynamics and Charge Storage in Ionic Liquid Supercapacitors. Journal of the American Chemical Society, 2015, 137, 7231-7242.	13.7	182
9	Computer simulations of ionic liquids at electrochemical interfaces. Physical Chemistry Chemical Physics, 2013, 15, 15781.	2.8	148
10	Imidazolium Ionic Liquid Interfaces with Vapor and Graphite: Interfacial Tension and Capacitance from Coarse-Grained Molecular Simulations. Journal of Physical Chemistry C, 2011, 115, 16613-16618.	3.1	139
11	Charge Fluctuations in Nanoscale Capacitors. Physical Review Letters, 2013, 111, 106102.	7.8	129
12	New Coarse-Grained Models of Imidazolium Ionic Liquids for Bulk and Interfacial Molecular Simulations. Journal of Physical Chemistry C, 2012, 116, 7687-7693.	3.1	126
13	Influence of solvation on the structural and capacitive properties of electrical double layer capacitors. Electrochimica Acta, 2013, 101, 262-271.	5.2	96
14	New Insights into the Structure of Nanoporous Carbons from NMR, Raman, and Pair Distribution Function Analysis. Chemistry of Materials, 2015, 27, 6848-6857.	6.7	88
15	Towards an atomistic understanding of disordered carbon electrode materials. Chemical Communications, 2018, 54, 5988-5991.	4.1	84
16	Tracking Ionic Rearrangements and Interpreting Dynamic Volumetric Changes in Twoâ€Dimensional Metal Carbide Supercapacitors: A Molecular Dynamics Simulation Study. ChemSusChem, 2018, 11, 1892-1899.	6.8	50
17	Computational Insights into Charge Storage Mechanisms of Supercapacitors. Energy and Environmental Materials, 2020, 3, 235-246.	12.8	49
18	Carbons with Regular Pore Geometry Yield Fundamental Insights into Supercapacitor Charge Storage. ACS Central Science, 2019, 5, 1813-1823.	11.3	44

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19	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. ACS Applied Materials & Interfaces, 2020, 12, 1789-1798.	8.0	39
20	Stochasticity of Pores Interconnectivity in Liâ€“O₂ Batteries and its Impact on the Variations in Electrochemical Performance. Journal of Physical Chemistry Letters, 2018, 9, 791-797.	4.6	37
21	Effects of functional groups and anion size on the charging mechanisms in layered electrode materials. Energy Storage Materials, 2020, 33, 460-469.	18.0	36
22	Single Electrode Capacitances of Porous Carbons in Neat Ionic Liquid Electrolyte at 100Â°C: A Combined Experimental and Modeling Approach. Journal of the Electrochemical Society, 2015, 162, A5091-A5095.	2.9	32
23	Thermal conductivity of ionic systems from equilibrium molecular dynamics. Journal of Physics Condensed Matter, 2011, 23, 102101.	1.8	30
24	Lattice simulation method to model diffusion and NMR spectra in porous materials. Journal of Chemical Physics, 2015, 142, 094701.	3.0	28
25	Structural Characterization of the Li-Ion Battery Cathode Materials LiTi_xMn_{2â€“x}O₄ (0.2 â‰¤ x â‰¤ 1.5): A Combined Experimental ⁷Li NMR and First-Principles Study. Chemistry of Materials, 2018, 30, 817-829.	6.7	27
26	Internal mobilities and diffusion in an ionic liquid mixture. Physical Chemistry Chemical Physics, 2010, 12, 14109.	2.8	24
27	NMR studies of adsorption and diffusion in porous carbonaceous materials. Progress in Nuclear Magnetic Resonance Spectroscopy, 2021, 124-125, 57-84.	7.5	19
28	Carbonâ€“carbon supercapacitors: Beyond the average pore size or how electrolyte confinement and inaccessible pores affect the capacitance. Journal of Chemical Physics, 2021, 155, 184703.	3.0	17
29	Text mining assisted review of the literature on Li-O₂ batteries. JPhys Materials, 2019, 2, 044004.	4.2	16
30	On the development of an original mesoscopic model to predict the capacitive properties of carbon-carbon supercapacitors. Electrochimica Acta, 2019, 327, 135022.	5.2	16
31	Importance of Incorporating Explicit 3D-Resolved Electrode Mesostructures in Liâ€“O₂ Battery Models. ACS Applied Energy Materials, 2018, 1, 6433-6441.	5.1	14
32	Elucidating Curvature-Capacitance Relationships in Carbon-Based Supercapacitors. Physical Review Letters, 2022, 128, 086001.	7.8	14
33	Local Distortions and Dynamics in Hydrated Y-Doped BaZrO₃. Journal of Physical Chemistry C, 2020, 124, 16689-16701.	3.1	12
34	Simulations of Ionic Liquids Confined in Surface-Functionalized Nanoporous Carbons: Implications for Energy Storage. ACS Applied Nano Materials, 2021, 4, 4007-4015.	5.0	12
35	Carbon electrodes for energy storage: general discussion. Faraday Discussions, 2014, 172, 239-260.	3.2	11
36	Probing and Interpreting the Porosity and Tortuosity Evolution of Li-O₂ Cathodes on Discharge through a Combined Experimental and Theoretical Approach. Journal of Physical Chemistry C, 2021, 125, 4955-4967.	3.1	11

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37	Efficient prediction of nucleus independent chemical shifts for polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2020, 22, 13746-13755.	2.8	10
38	Mesoscopic simulations of the in situ NMR spectra of porous carbon based supercapacitors: electronic structure and adsorbent reorganisation effects. Physical Chemistry Chemical Physics, 2021, 23, 15925-15934.	2.8	4
39	Tracking Ionic Rearrangements and Interpreting Dynamic Volumetric Changes in Twoâ€Dimensional Metal Carbide Supercapacitors: A Molecular Dynamics Simulation Study. ChemSusChem, 2018, 11, 1889-1889.	6.8	3
40	Molecular Dynamics Simulations of Electrochemical Energy Storage Devices. Green Energy and Technology, 2016, , 61-89.	0.6	3