Jean-Marc Leyssale

List of Publications by Year
in descending order

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29 papers	623 citations	516710 16 h-index	580821 25 g-index
30 all docs	30 docs citations	30 times ranked	709 citing authors

#	Article	IF	Citations
1	Atomic-scale mechanism of carbon nucleation from a deep crustal fluid by replica exchange reactive molecular dynamics simulation. Geochimica Et Cosmochimica Acta, 2022, 329, 106-118.	3.9	4
2	Texture, Nanotexture, and Structure of Carbon Nanotube-Supported Carbon Cones. ACS Nano, 2022, 16, 9287-9296.	14.6	7
3	Mechanisms of elastic softening in highly anisotropic carbons under in-plane compression/indentation. Carbon, 2022, 197, 425-434.	10.3	5
4	¹³C NMR Parameters of Disordered Carbons: Atomistic Simulations, DFT Calculations, and Experimental Results. Journal of Physical Chemistry C, 2020, 124, 12784-12793.	3.1	6
5	Timescale prediction of complex multi-barrier pathways using flux sampling molecular dynamics and 1D kinetic integration: Application to cellulose dehydration. Journal of Chemical Physics, 2020, 152, 024123.	3.0	6
6	Simulating the Geological Fate of Terrestrial Organic Matter: Lignin vs Cellulose. Energy & Fuels, 2020, 34, 1537-1547.	5.1	15
7	Methane Diffusion in a Flexible Kerogen Matrix. Journal of Physical Chemistry B, 2019, 123, 5635-5640.	2.6	30
8	Evolution of Threshold Displacement Energy in Irradiated Graphite. Physical Review Applied, 2018, 10, .	3.8	13
9	Poroelasticity of Methane-Loaded Mature and Immature Kerogen from Molecular Simulations. Langmuir, 2018, 34, 13766-13780.	3.5	35
10	A time-dependent atomistic reconstruction of severe irradiation damage and associated property changes in nuclear graphite. Carbon, 2017, 120, 111-120.	10.3	23
11	Matricial inclusion of AlN and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0008.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mi>Al</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:mrow></mml:math> nanoparticles in C/C composites from aqueous growth and ceramization at the pre-densified stage. Ceramics International, 2017, 43, 17015-17021.	4.8	0
12	From cellulose to kerogen: molecular simulation of a geological process. Chemical Science, 2017, 8, 8325-8335.	7.4	37
13	Mechanism of strength reduction along the graphenization pathway. Science Advances, 2015, 1, e1501009.	10.3	16
14	On the prediction of grapheneâ€™s elastic properties with reactive empirical bond order potentials. Carbon, 2015, 89, 176-187.	10.3	32
15	Carbonâ€“ceramic (AlN) interfaces from liquid quench ab initio molecular dynamics simulations. Molecular Simulation, 2014, 40, 160-168.	2.0	4
16	A Large-Scale Molecular Dynamics Study of the Divacancy Defect in Graphene. Journal of Physical Chemistry C, 2014, 118, 8200-8216.	3.1	40
17	Structure of an Amorphous Boron Carbide Film: An Experimental and Computational Approach. Chemistry of Materials, 2013, 25, 2618-2629.	6.7	40
18	Rippled nanocarbons from periodic arrangements of reordered bivacancies in graphene or nanotubes. Journal of Chemical Physics, 2012, 136, 124705.	3.0	7

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19	Microstructure of pyrocarbons from pair distribution function analysis using neutron diffraction. Carbon, 2012, 50, 1563-1573.	10.3	30
20	Theoretical Study of the Decomposition of BCl₃ Induced by a H Radical. Journal of Physical Chemistry A, 2011, 115, 4786-4797.	2.5	8
21	Reaction Mechanism for the Thermal Decomposition of BCl₃/CH₄/H₂ Gas Mixtures. Journal of Physical Chemistry A, 2011, 115, 11579-11588.	2.5	9
22	Hindered rotor models with variable kinetic functions for accurate thermodynamic and kinetic predictions. Journal of Chemical Physics, 2010, 133, 154112.	3.0	13
23	An image-guided atomistic reconstruction of pyrolytic carbons. Applied Physics Letters, 2009, 95, .	3.3	34
24	Molecular Dynamics of Carbon Dioxide, Methane and Their Mixtures in a Zeolite Possessing Two Independent Pore Networks as Revealed by Computer Simulations. Journal of Physical Chemistry B, 2009, 113, 13761-13767.	2.6	18
25	Sorption Thermodynamics of CO2, CH4, and Their Mixtures in the ITQ-1 Zeolite as Revealed by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 22742-22753.	2.6	39
26	Computer simulation of Clâ" hydration in anionâ€"water clusters. Chemical Physics, 2005, 310, 97-107.	1.9	57
27	Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. Journal of Chemical Physics, 2005, 122, 104510.	3.0	36
28	Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. Journal of Chemical Physics, 2005, 122, 184518.	3.0	27
29	Reorganization and Growth of Metastable Î±-N2Critical Nuclei into Stable Î²-N2Crystals. Journal of the American Chemical Society, 2004, 126, 12286-12287.	13.7	32