Jean-Marc Leyssale

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5887599/publications.pdf

Version: 2024-02-01

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	Computer simulation of Clâ˜ hydration in anionâ€“water clusters. Chemical Physics, 2005, 310, 97-107.	1.9	57
2	Structure of an Amorphous Boron Carbide Film: An Experimental and Computational Approach. Chemistry of Materials, 2013, 25, 2618-2629.	6.7	40
3	A Large-Scale Molecular Dynamics Study of the Divacancy Defect in Graphene. Journal of Physical Chemistry C, 2014, 118, 8200-8216.	3.1	40
4	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
5	From cellulose to kerogen: molecular simulation of a geological process. Chemical Science, 2017, 8, 8325-8335.	7.4	37
6	Atomistic simulation of the homogeneous nucleation and of the growth of N2 crystallites. Journal of Chemical Physics, 2005, 122, 104510.	3.0	36
7	Poroelasticity of Methane-Loaded Mature and Immature Kerogen from Molecular Simulations. Langmuir, 2018, 34, 13766-13780.	3.5	35
8	An image-guided atomistic reconstruction of pyrolytic carbons. Applied Physics Letters, 2009, 95, .	3.3	34
9	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
10	On the prediction of grapheneâ€™s elastic properties with reactive empirical bond order potentials. Carbon, 2015, 89, 176-187.	10.3	32
11	Microstructure of pyrocarbons from pair distribution function analysis using neutron diffraction. Carbon, 2012, 50, 1563-1573.	10.3	30
12	Methane Diffusion in a Flexible Kerogen Matrix. Journal of Physical Chemistry B, 2019, 123, 5635-5640.	2.6	30
13	Molecular simulation of the homogeneous crystal nucleation of carbon dioxide. Journal of Chemical Physics, 2005, 122, 184518.	3.0	27
14	A time-dependent atomistic reconstruction of severe irradiation damage and associated property changes in nuclear graphite. Carbon, 2017, 120, 111-120.	10.3	23
15	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
16	Mechanism of strength reduction along the graphenization pathway. Science Advances, 2015, 1, e1501009.	10.3	16
17	Simulating the Geological Fate of Terrestrial Organic Matter: Lignin vs Cellulose. Energy & Fuels, 2020, 34, 1537-1547.	5.1	15
18	Hindered rotor models with variable kinetic functions for accurate thermodynamic and kinetic predictions. Journal of Chemical Physics, 2010, 133, 154112.	3.0	13

#	Article	IF	Citations
19	Evolution of Threshold Displacement Energy in Irradiated Graphite. Physical Review Applied, 2018, 10, .	3.8	13
20	Reaction Mechanism for the Thermal Decomposition of BCl₃/CH₄/H₂ Gas Mixtures. Journal of Physical Chemistry A, 2011, 115, 11579-11588.	2.5	9
21	Theoretical Study of the Decomposition of BCl₃ Induced by a H Radical. Journal of Physical Chemistry A, 2011, 115, 4786-4797.	2.5	8
22	Rippled nanocarbons from periodic arrangements of reordered bivacancies in graphene or nanotubes. Journal of Chemical Physics, 2012, 136, 124705.	3.0	7
23	Texture, Nanotexture, and Structure of Carbon Nanotube-Supported Carbon Cones. ACS Nano, 2022, 16, 9287-9296.	14.6	7
24	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
25	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
26	Mechanisms of elastic softening in highly anisotropic carbons under in-plane compression/indentation. Carbon, 2022, 197, 425-434.	10.3	5
27	Carbonâ€“ceramic (AlN) interfaces from liquid quench ab initio molecular dynamics simulations. Molecular Simulation, 2014, 40, 160-168.	2.0	4
28	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
29	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:mo></mml:mo><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></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