Yongsheng Leng

List of Publications by Year
in descending order

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66	1,766	218677	276875
papers	citations	26 h-index	41 g-index

67	67	67	2031
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Fluidity of Hydration Layers Nanoconfined between Mica Surfaces. Physical Review Letters, 2005, 94, 026101.	7.8	169
2	Hydration structure of water confined between mica surfaces. Journal of Chemical Physics, 2006, 124, 074711.	3.0	105
3	Hydration Force between Mica Surfaces in Aqueous KCl Electrolyte Solution. Langmuir, 2012, 28, 5339-5349.	3.5	90
4	Molecular Dynamics Simulations of Polyamide Membrane, Calcium Alginate Gel, and Their Interactions in Aqueous Solution. Langmuir, 2014, 30, 9098-9106.	3.5	82
5	Hydrated Polyamide Membrane and Its Interaction with Alginate: A Molecular Dynamics Study. Langmuir, 2013, 29, 11600-11608.	3.5	73
6	Theory of piezotronics and piezo-phototronics. MRS Bulletin, 2018, 43, 928-935.	3.5	66
7	Atomic indentation and friction of self-assembled monolayers by hybrid molecular simulations. Journal of Chemical Physics, 2000, 113, 8800-8806.	3.0	60
8	Dynamic Simulations of Adhesion and Friction in Chemical Force Microscopy. Journal of the American Chemical Society, 2002, 124, 11764-11770.	13.7	57
9	Molecular dynamics simulations of stretched gold nanowires: The relative utility of different semiempirical potentials. Journal of Chemical Physics, 2007, 126, 144707.	3.0	57
10	Molecular Understanding of CO₂ and H₂O in a Montmorillonite Clay Interlayer under CO₂ Geological Sequestration Conditions. Journal of Physical Chemistry C, 2016, 120, 2642-2654.	3.1	47
11	Molecular Simulations of the Hydration Behavior of a Zwitterion Brush Array and Its Antifouling Property in an Aqueous Environment. Langmuir, 2018, 34, 2245-2257.	3.5	46
12	Phase transition in two-dimensional tellurene under mechanical strain modulation. Nano Energy, 2019, 58, 202-210.	16.0	43
13	Self-Assembly of 1,4-Benzenedithiolate/Tetrahydrofuran on a Gold Surface:Â A Monte Carlo Simulation Study. Langmuir, 2006, 22, 4116-4124.	3.5	42
14	Stick-Slip Friction and Energy Dissipation in Boundary Lubrication. Physical Review Letters, 2011, 107, 147801.	7.8	42
15	Computational chemistry for molecular electronics. Computational Materials Science, 2003, 28, 321-341.	3.0	41
16	Molecular Dynamics Simulations of a Poly(ethylene glycol)-Grafted Polyamide Membrane and Its Interaction with a Calcium Alginate Gel. Langmuir, 2016, 32, 4424-4433.	3.5	41
17	Molecular simulations of stretching gold nanowires in solvents. Nanotechnology, 2007, 18, 424007.	2.6	39
18	Ultrafast photoinduced band splitting and carrier dynamics in chiral tellurium nanosheets. Nature Communications, 2020, 11, 3991.	12.8	39

#	Article	IF	Citations
19	Shear dynamics of hydration layers. Journal of Chemical Physics, 2006, 125, 104701.	3.0	38
20	Tip-Based Hybrid Simulation Study of Frictional Properties of Self-Assembled Monolayers:â€‰ Effects of Chain Length, Terminal Group, Scan Direction, and Scan Velocity. Langmuir, 2003, 19, 9742-9747.	3.5	37
21	Molecular Simulations on the Structure and Dynamics of Waterâ€“Methane Fluids between Na-Montmorillonite Clay Surfaces at Elevated Temperature and Pressure. Journal of Physical Chemistry C, 2013, 117, 14061-14069.	3.1	35
22	Squeezing and stickâ€“slip friction behaviors of lubricants in boundary lubrication. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6560-6565.	7.1	31
23	Structure and Dynamics of a Benzenedithiol Monolayer on a Au(111) Surface. Journal of Physical Chemistry B, 2003, 107, 11940-11950.	2.6	27
24	Interaction between benzenedithiolate and gold: Classical force field for chemical bonding. Journal of Chemical Physics, 2005, 122, 244721.	3.0	27
25	Hydration force and dynamic squeeze-out of hydration water under subnanometer confinement. Journal of Physics Condensed Matter, 2008, 20, 354017.	1.8	27
26	Unbinding of the streptavidin-biotin complex by atomic force microscopy: A hybrid simulation study. Journal of Chemical Physics, 2006, 125, 104905.	3.0	26
27	Methane Aqueous Fluids in Montmorillonite Clay Interlayer under Near-Surface Geological Conditions: A Grand Canonical Monte Carlo and Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2014, 118, 10956-10965.	2.6	24
28	On the metal/ZnO contacts in a sliding-bending piezoelectric nanogenerator. Nano Energy, 2018, 50, 291-297.	16.0	23
29	Title is missing!. Journal of Materials Science, 2000, 35, 2061-2067.	3.7	22
30	Molecular Simulation Studies on the Elongation of Gold Nanowires in Benzenedithiol. Journal of Physical Chemistry C, 2010, 114, 10365-10372.	3.1	22
31	Gold/Benzenedithiolate/Gold Molecular Junction: A Driven Dynamics Simulation on Structural Evolution and Breaking Force under Pulling. Journal of Physical Chemistry C, 2015, 119, 15216-15223.	3.1	22
32	Effect of Layer Charge on CO₂ and H₂O Intercalations in Swelling Clays. Langmuir, 2016, 32, 11366-11374.	3.5	22
33	Force oscillation and phase transition of simple fluids under confinement. Physical Review E, 2010, 82, 040501.	2.1	21
34	The impact of radicals in cold atmospheric plasma on the structural modification of gap junction: a reactive molecular dynamics study. International Journal of Smart and Nano Materials, 2019, 10, 144-155.	4.2	21
35	Rate-Dependent Energy Release Mechanism of Gold Nanowires under Elongation. Journal of the American Chemical Society, 2008, 130, 17907-17912.	13.7	19
36	Water structures near charged (100) and (111) silicon surfaces. Applied Physics Letters, 2009, 94, .	3.3	18

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37	Solvation force simulations in atomic force microscopy. Journal of Chemical Physics, 2014, 140, 214702.	3.0	16
38	Hydrophobic Drying and Hysteresis at Different Length Scales by Molecular Dynamics Simulations. Langmuir, 2012, 28, 3152-3158.	3.5	14
39	Measurement of Single-Molecule Forces in Cholesterol and Cyclodextrin Hostâ€“Guest Complexes. Journal of Physical Chemistry B, 2021, 125, 11112-11121.	2.6	13
40	Molecular dynamics simulations of the stable structures of single atomic contacts in gold nanojunctions. Physical Review B, 2011, 84, .	3.2	12
41	A comparative study by the grand canonical Monte Carlo and molecular dynamics simulations on the squeezing behavior of nanometers confined liquid films. Journal of Chemical Physics, 2013, 139, 074704.	3.0	11
42	Contact stiffness and damping of liquid films in dynamic atomic force microscope. Journal of Chemical Physics, 2016, 144, 154702.	3.0	11
43	Computational simulations of solvation force and squeezing out of dodecane chain molecules in an atomic force microscope. Journal of Chemical Physics, 2017, 147, 054705.	3.0	10
44	Molecular Understanding of Ion Effect on Polyzwitterion Conformation in an Aqueous Environment. Langmuir, 2020, 36, 7648-7657.	3.5	10
45	A Molecular Dynamics Simulations Study of the Influence of Prestrain on the Pop-In Behavior and Indentation Size Effect in Cu Single Crystals. Materials, 2021, 14, 5220.	2.9	10
46	Will Polycrystalline Platinum Tip Sliding on a Gold(111) Surface Produce Regular Stickâ€“Slip Friction?. Langmuir, 2022, 38, 6808-6816.	3.5	9
47	Comparative studies on the structure and diffusion dynamics of aqueous and nonpolar liquid films under nanometers confinement. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 034007.	2.0	7
48	How alginate monomers contribute to organic fouling on polyamide membrane surfaces?. Journal of Membrane Science, 2022, 643, 120078.	8.2	7
49	Nano-tribology through molecular dynamics simulations. Science in China Series A: Mathematics, 2001, 44, 1049-1055.	0.5	6
50	Spanning Time Scales in Dynamic Simulations of Atomic-Scale Friction. Tribology Letters, 2001, 11, 111-115.	2.6	6
51	Dissipative process in atomic force microscopy. Physical Review B, 2001, 64, .	3.2	4
52	Molecular Simulation Study of Piezoelectric Potential Distribution in a ZnO Nanowire under Mechanical Bending. MRS Advances, 2017, 2, 3433-3439.	0.9	4
53	On the shear dilation of polycrystalline lubricant films in boundary lubricated contacts. Journal of Chemical Physics, 2020, 152, 104708.	3.0	4
54	On the asymptotic expressions of critical energy barrier in Prandtl-Tomlinson model. International Journal of Smart and Nano Materials, 2019, 10, 107-115.	4.2	3

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55	Molecular simulation of metal-ZnO contact in ZnO piezoelectric nanogenerator. , 2013, , .		2
56	Computational Simulations of Nanoconfined Argon Film through Adsorptionâ€“Desorption in a Uniform Slit Pore. Coatings, 2021, 11, 177.	2.6	2
57	Hydration Structure and Shear Viscosity of Water Nanoconfined Between Mica Surfaces. , 2006, , 505.		1
58	Surface force apparatus and its application to research of the surface contact. Science Bulletin, 1999, 44, 992-995.	1.7	0
59	Integrated multiscale modeling of molecular computing devices. Journal of Physics: Conference Series, 2005, 16, 269-272.	0.4	0
60	Molecular Dynamics Simulation of Water and Ion Profiles Near Charged (100) and (111) Silicon Surfaces. , 2008, , .		0
61	Driven Dynamics of Long-Time Bond-Breaking Events. Langmuir, 2019, 35, 16961-16968.	3.5	0
62	Molecular Dynamics Simulations of Water and Ion Structures Near Charged Surfaces. , 2007, , .		0
63	Molecular Dynamics Simulation of Phase Transition and Solvation Force Oscillation of Simple Nanoconfined Fluids. , 2013, , 2305-2309.		0
64	Molecular Dynamics Simulation of Hydrophobic Interaction and Hysteresis at Different Length Scales. , 2013, , 2301-2305.		0
65	Direct Measurement of Intermolecular Mechanical Force for Nonspecific Interactions between Small Molecules. Journal of Physical Chemistry Letters, 2021, 12, 11316-11322.	4.6	0
66	Nucleation of Frank Dislocation during the Squeeze-Out Process in Boundary Lubrication: A Molecular Dynamics Study. Materials, 2022, 15, 997.	2.9	0