Lianchi Liu

List of Publications by Year
in descending order

11	838	933447 10	1281871 11
papers	citations	h-index	g-index

11	11	11	917
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ReaxFF-lg: Correction of the ReaxFF Reactive Force Field for London Dispersion, with Applications to the Equations of State for Energetic Materials. Journal of Physical Chemistry A, 2011, 115, 11016-11022.	2.5	401
2	Mechanism and Kinetics for the Initial Steps of Pyrolysis and Combustion of 1,6-Dicyclopropane-2,4-hexyne from ReaxFF Reactive Dynamics. Journal of Physical Chemistry A, 2011, 115, 4941-4950.	2.5	103
3	Development of a ReaxFF Reactive Force Field for Ettringite and Study of its Mechanical Failure Modes from Reactive Dynamics Simulations. Journal of Physical Chemistry A, 2012, 116, 3918-3925.	2.5	79
4	Semi-ionic Model for Metal Oxides and Their Interfaces with Organic Molecules. Journal of Physical Chemistry C, 2007, 111, 10610-10617.	3.1	74
5	Molecular Dynamics Simulations of Methanol to Olefin Reactions in HZSM-5 Zeolite Using a ReaxFF Force Field. Journal of Physical Chemistry C, 2012, 116, 7029-7039.	3.1	44
6	Toward a Process-Based Molecular Model of SiC Membranes. 1. Development of a Reactive Force Field. Journal of Physical Chemistry C, 2013, 117, 3308-3319.	3.1	39
7	Simulation of NH₃ Temperature-Programmed Desorption Curves Using an ab Initio Force Field. Journal of Physical Chemistry C, 2009, 113, 16051-16057.	3.1	28
8	Toward a Process-Based Molecular Model of SiC Membranes. 2. Reactive Dynamics Simulation of the Pyrolysis of Polymer Precursor To Form Amorphous SiC. Journal of Physical Chemistry C, 2013, 117, 3320-3329.	3.1	24
9	Structures, Mechanisms, and Kinetics of Ammoxidation and Selective Oxidation of Propane Over the M2 Phase of MoVNbTeO Catalysts. Topics in Catalysis, 2011, 54, 659-668.	2.8	22
10	ReaxFF reactive molecular dynamics on silicon pentaerythritol tetranitrate crystal validates the mechanism for the colossal sensitivity. Physical Chemistry Chemical Physics, 2014, 16, 23779-23791.	2.8	21
11	Prediction of adsorption of small molecules in porous materials based on ab initio force field method. Science in China Series B: Chemistry, 2008, 51, 760-767.	0.8	3