

# Xiang-Yang Liu

## List of Publications by Citations

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31  
papers

519  
citations

14  
h-index

22  
g-index

32  
ext. papers

591  
ext. citations

4.5  
avg, IF

3.99  
L-index

#	Paper	IF	Citations
31	Revisiting the Al/Al <sub>2</sub> O <sub>3</sub> Interface: coherent interfaces and misfit accommodation. <i>Scientific Reports</i> , <b>2014</b> , 4, 4485	4.9	55
30	Development of a multiscale thermal conductivity model for fission gas in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , <b>2016</b> , 469, 89-98	3.3	50
29	The influence of dilute heats of mixing on the atomic structures, defect energetics and mechanical properties of fcc/bcc interfaces. <i>Acta Materialia</i> , <b>2010</b> , 58, 4549-4557	8.4	43
28	First-principles DFT modeling of nuclear fuel materials. <i>Journal of Materials Science</i> , <b>2012</b> , 47, 7367-7384	4.3	42
27	First-principles density functional theory study of generalized stacking faults in TiN and MgO. <i>Philosophical Magazine</i> , <b>2014</b> , 94, 464-475	1.6	28
26	Liquid-phase thermodynamics and structures in the Cu/Ni binary system. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2013</b> , 21, 025005	2	25
25	Growth and Stress-induced Transformation of Zinc blende AlN Layers in Al-AlN-TiN Multilayers. <i>Scientific Reports</i> , <b>2015</b> , 5, 18554	4.9	23
24	Crack tip plasticity in single crystal UO <sub>2</sub> : Atomistic simulations. <i>Journal of Nuclear Materials</i> , <b>2012</b> , 430, 96-105	3.3	23
23	Molecular dynamics study of fission gas bubble nucleation in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , <b>2015</b> , 462, 8-14	3.3	21
22	Review: mechanical behavior of metal/ceramic interfaces in nanolayered composites: Experiments and modeling. <i>Journal of Materials Science</i> , <b>2018</b> , 53, 5562-5583	4.3	20
21	Heterotwin formation during growth of nanolayered Al-TiN composites. <i>Applied Physics Letters</i> , <b>2010</b> , 96, 093113	3.4	19
20	Behavior of Vacancies and Interstitials at Semicoherent Interfaces. <i>Jom</i> , <b>2013</b> , 65, 374-381	2.1	18
19	Investigation of structure and composition control over active dissolution of Fe/C binary metallic waste forms by off-lattice kinetic Monte Carlo simulation. <i>Journal of Nuclear Materials</i> , <b>2013</b> , 434, 382-388	3.3	17
18	Thermodynamics of fission products in dispersion fuel designs: First-principles modeling of defect behavior in bulk and at interfaces. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2010</b> , 268, 3014-3017	4.2	17
17	First-principles prediction of the thermodynamic stability of xenon in monoclinic, tetragonal, and yttrium-stabilized cubic ZrO <sub>2</sub> . <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	14
16	New helium bubble growth mode at a symmetric grain-boundary in tungsten: accelerated molecular dynamics study. <i>Materials Research Letters</i> , <b>2018</b> , 6, 522-530	7.4	13
15	Perfect Strain Relaxation in Metamorphic Epitaxial Aluminum on Silicon through Primary and Secondary Interface Misfit Dislocation Arrays. <i>ACS Nano</i> , <b>2018</b> , 12, 6843-6850	16.7	12

14	Mechanically controlling the reversible phase transformation from zinc blende to wurtzite in AlN. <i>Materials Research Letters</i> , <b>2017</b> , 5, 426-432	7.4	11
13	Revisiting the diffusion mechanism of helium in UO <sub>2</sub> : A DFT+U study. <i>Journal of Nuclear Materials</i> , <b>2018</b> , 498, 373-377	3.3	11
12	First-Principles and Kinetic Monte Carlo Simulation Studies of the Reactivity of Tc(0001), MoTc(111) and MoTc(110) Surfaces. <i>Journal of the Electrochemical Society</i> , <b>2014</b> , 161, C83-C88	3.9	10
11	First-principles study of fission product (Xe, Cs, Sr) incorporation and segregation in alkaline earth metal oxides, HfO <sub>2</sub> , and the MgO-HfO <sub>2</sub> interface. <i>Journal of Physics Condensed Matter</i> , <b>2009</b> , 21, 045403	1.8	10
10	Lanthanum energetics in cubic ZrO <sub>2</sub> and UO <sub>2</sub> from DFT and DFT + U studies. <i>Journal of Nuclear Materials</i> , <b>2011</b> , 414, 217-220	3.3	9
9	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 46296-46305	9.5	7
8	Data-enabled structure-property mappings for lanthanide-activated inorganic scintillators. <i>Journal of Materials Science</i> , <b>2019</b> , 54, 8361-8380	4.3	5
7	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites <b>2012</b> ,		5
6	Screw dislocation impingement and slip transfer at fcc-bcc semicoherent interfaces. <i>Scripta Materialia</i> , <b>2021</b> , 201, 113977	5.6	4
5	Dissociated vacancies and screw dislocations in MgO and UO: atomistic modeling and linear elasticity analysis. <i>Scientific Reports</i> , <b>2019</b> , 9, 6499	4.9	3
4	Accurately predicting optical properties of rare-earth, aluminate scintillators: influence of electron-phonon correlation. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 7292-7301	7.1	3
3	First principles approach to ionicity of fragments. <i>Chemical Physics</i> , <b>2015</b> , 448, 26-33	2.3	1
2	Interphase Defects, Structures, and Phase Stability. <i>Jom</i> , <b>2013</b> , 65, 358-359	2.1	
1	Atomistic modeling of plastic deformation in B <sub>2</sub> -FeAl/Al nanolayered composites. <i>Journal of Materials Science</i> , <b>2021</b> , 56, 17080-17095	4.3	