Xiang-Yang Liu

List of Publications by Year in Descending Order

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	Accurately predicting optical properties of rare-earth, aluminate scintillators: influence of electron□hole correlation. *Journal of Materials Chemistry C*, **2021**, 9, 7292-7301	7.1	3
30	Atomistic modeling of plastic deformation in B2-FeAl/Al nanolayered composites. *Journal of Materials Science*, **2021**, 56, 17080-17095	4.3	
29	Screw dislocation impingement and slip transfer at fcc-bcc semicoherent interfaces. *Scripta Materialia*, **2021**, 201, 113977	5.6	4
28	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. *ACS Applied Materials & Interfaces*, **2020**, 12, 46296-46305	9.5	7
27	Dissociated vacancies and screw dislocations in MgO and UO: atomistic modeling and linear elasticity analysis. *Scientific Reports*, **2019**, 9, 6499	4.9	3
26	Data-enabled structure□property mappings for lanthanide-activated inorganic scintillators. *Journal of Materials Science*, **2019**, 54, 8361-8380	4.3	5
25	Perfect Strain Relaxation in Metamorphic Epitaxial Aluminum on Silicon through Primary and Secondary Interface Misfit Dislocation Arrays. *ACS Nano*, **2018**, 12, 6843-6850	16.7	12
24	New helium bubble growth mode at a symmetric grain-boundary in tungsten: accelerated molecular dynamics study. *Materials Research Letters*, **2018**, 6, 522-530	7.4	13
23	Revisiting the diffusion mechanism of helium in UO2: A DFT+U study. *Journal of Nuclear Materials*, **2018**, 498, 373-377	3.3	11
22	Review: mechanical behavior of metal/ceramic interfaces in nanolayered composites□experiments and modeling. *Journal of Materials Science*, **2018**, 53, 5562-5583	4.3	20
21	Mechanically controlling the reversible phase transformation from zinc blende to wurtzite in AlN. *Materials Research Letters*, **2017**, 5, 426-432	7.4	11
20	Development of a multiscale thermal conductivity model for fission gas in UO2. *Journal of Nuclear Materials*, **2016**, 469, 89-98	3.3	50
19	First principles approach to ionicity of fragments. *Chemical Physics*, **2015**, 448, 26-33	2.3	1
18	Molecular dynamics study of fission gas bubble nucleation in UO2. *Journal of Nuclear Materials*, **2015**, 462, 8-14	3.3	21
17	Growth and Stress-induced Transformation of Zinc blende AlN Layers in Al-AlN-TiN Multilayers. *Scientific Reports*, **2015**, 5, 18554	4.9	23
16	Revisiting the Al/Al□□ interface: coherent interfaces and misfit accommodation. *Scientific Reports*, **2014**, 4, 4485	4.9	55
15	First-principles density functional theory study of generalized stacking faults in TiN and MgO. *Philosophical Magazine*, **2014**, 94, 464-475	1.6	28

List of Publications

14	First-Principles and Kinetic Monte Carlo Simulation Studies of the Reactivity of Tc(0001), MoTc(111) and MoTc(110) Surfaces. *Journal of the Electrochemical Society*, **2014**, 161, C83-C88	3.9	10
13	Interphase Defects, Structures, and Phase Stability. *Jom*, **2013**, 65, 358-359	2.1	
12	Behavior of Vacancies and Interstitials at Semicoherent Interfaces. *Jom*, **2013**, 65, 374-381	2.1	18
11	Investigation of structure and composition control over active dissolution of Fe□c binary metallic waste forms by off-lattice kinetic Monte Carlo simulation. *Journal of Nuclear Materials*, **2013**, 434, 382-388	3.3	17
10	Liquid-phase thermodynamics and structures in the Cu□b binary system. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 025005	2	25
9	First-principles DFT modeling of nuclear fuel materials. *Journal of Materials Science*, **2012**, 47, 7367-7384	4.3	42
8	Crack tip plasticity in single crystal UO2: Atomistic simulations. *Journal of Nuclear Materials*, **2012**, 430, 96-105	3.3	23
7	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites **2012**,		5
6	Lanthanum energetics in cubic ZrO2 and UO2 from DFT and DFT + U studies. *Journal of Nuclear Materials*, **2011**, 414, 217-220	3.3	9
5	First-principles prediction of the thermodynamic stability of xenon in monoclinic, tetragonal, and yttrium-stabilized cubic ZrO2. *Physical Review B*, **2011**, 83,	3.3	14
4	Heterotwin formation during growth of nanolayered Al-TiN composites. *Applied Physics Letters*, **2010**, 96, 093113	3.4	19
3	Thermodynamics of fission products in dispersion fuel designs □First-principles modeling of defect behavior in bulk and at interfaces. *Nuclear Instruments & Methods in Physics Research B*, **2010**, 268, 3014-3017	1.2	17
2	The influence of dilute heats of mixing on the atomic structures, defect energetics and mechanical properties of fcc□bcc interfaces. *Acta Materialia*, **2010**, 58, 4549-4557	8.4	43
1	First-principles study of fission product (Xe, Cs, Sr) incorporation and segregation in alkaline earth metal oxides, HfO(2), and the MgO-HfO(2) interface. *Journal of Physics Condensed Matter*, **2009**, 21, 045403	1.8	10