

Xiang-Yang Liu

List of Publications by Year in descending order

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32
papers

658
citations

516215

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all docs

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docs citations

32
times ranked

827
citing authors

#	ARTICLE	IF	CITATIONS
1	Revisiting the Al/Al ₂ O ₃ Interface: Coherent Interfaces and Misfit Accommodation. <i>Scientific Reports</i> , 2014, 4, 4485.	1.6	78
2	Development of a multiscale thermal conductivity model for fission gas in UO ₂ . <i>Journal of Nuclear Materials</i> , 2016, 469, 89-98.	1.3	63
3	First-principles DFT modeling of nuclear fuel materials. <i>Journal of Materials Science</i> , 2012, 47, 7367-7384.	1.7	47
4	The influence of dilute heats of mixing on the atomic structures, defect energetics and mechanical properties of fcc/bcc interfaces. <i>Acta Materialia</i> , 2010, 58, 4549-4557.	3.8	45
5	Liquid-phase thermodynamics and structures in the Cu-Nb binary system. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2013, 21, 025005.	0.8	32
6	First-principles density functional theory study of generalized stacking faults in TiN and MgO. <i>Philosophical Magazine</i> , 2014, 94, 464-475.	0.7	32
7	Review: mechanical behavior of metal/ceramic interfaces in nanolayered composites—experiments and modeling. <i>Journal of Materials Science</i> , 2018, 53, 5562-5583.	1.7	31
8	Crack tip plasticity in single crystal UO ₂ : Atomistic simulations. <i>Journal of Nuclear Materials</i> , 2012, 430, 96-105.	1.3	29
9	Molecular dynamics study of fission gas bubble nucleation in UO ₂ . <i>Journal of Nuclear Materials</i> , 2015, 462, 8-14.	1.3	29
10	Growth and Stress-induced Transformation of Zinc blende AlN Layers in Al-AlN-TiN Multilayers. <i>Scientific Reports</i> , 2016, 5, 18554.	1.6	25
11	Heterotwin formation during growth of nanolayered Al-TiN composites. <i>Applied Physics Letters</i> , 2010, 96, .	1.5	24
12	New helium bubble growth mode at a symmetric grain-boundary in tungsten: accelerated molecular dynamics study. <i>Materials Research Letters</i> , 2018, 6, 522-530.	4.1	20
13	Behavior of Vacancies and Interstitials at Semicoherent Interfaces. <i>Jom</i> , 2013, 65, 374-381.	0.9	19
14	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 46296-46305.	4.0	19
15	Investigation of structure and composition control over active dissolution of Fe-Tc binary metallic waste forms by off-lattice kinetic Monte Carlo simulation. <i>Journal of Nuclear Materials</i> , 2013, 434, 382-388.	1.3	18
16	Thermodynamics of fission products in dispersion fuel designs—First-principles modeling of defect behavior in bulk and at interfaces. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2010, 268, 3014-3017.	0.6	17
17	Perfect Strain Relaxation in Metamorphic Epitaxial Aluminum on Silicon through Primary and Secondary Interface Misfit Dislocation Arrays. <i>ACS Nano</i> , 2018, 12, 6843-6850.	7.3	17
18	Mechanically controlling the reversible phase transformation from zinc blende to wurtzite in AlN. <i>Materials Research Letters</i> , 2017, 5, 426-432.	4.1	15

#	ARTICLE	IF	CITATIONS
19	Revisiting the diffusion mechanism of helium in UO ₂ : A DFT+U study. Journal of Nuclear Materials, 2018, 498, 373-377.	1.3	15
20	First-principles prediction of the thermodynamic stability of xenon in monoclinic, tetragonal, and yttrium-stabilized cubic ZrO ₂ . Physical Review B, 2011, 83, .	1.1	14
21	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.	1.3	11
22	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.	0.7	10
23	Lanthanum energetics in cubic ZrO ₂ and UO ₂ from DFT and DFT+U studies. Journal of Nuclear Materials, 2011, 414, 217-220.	1.3	10
24	Data-enabled structure-property mappings for lanthanide-activated inorganic scintillators. Journal of Materials Science, 2019, 54, 8361-8380.	1.7	9
25	Screw dislocation impingement and slip transfer at fcc-bcc semicoherent interfaces. Scripta Materialia, 2021, 201, 113977.	2.6	9
26	Accurately predicting optical properties of rare-earth, aluminate scintillators: influence of electron-hole correlation. Journal of Materials Chemistry C, 2021, 9, 7292-7301.	2.7	8
27	Nonequilibrium molecular dynamics simulations of shock wave propagation in nanolayered Cu/Nb nanocomposites. AIP Conference Proceedings, 2012, , .	0.3	6
28	Dissociated vacancies and screw dislocations in MgO and UO ₂ : atomistic modeling and linear elasticity analysis. Scientific Reports, 2019, 9, 6499.	1.6	4
29	First principles approach to ionicity of fragments. Chemical Physics, 2015, 448, 26-33.	0.9	1
30	Reduction of bright exciton lifetimes by radiation-induced disorder. Physical Review Materials, 2021, 5, .	0.9	1
31	Interphase Defects, Structures, and Phase Stability. Jom, 2013, 65, 358-359.	0.9	0
32	Atomistic modeling of plastic deformation in B ₂ -FeAl/Al nanolayered composites. Journal of Materials Science, 2021, 56, 17080-17095.	1.7	0