

Khang Hoang

List of Publications by Year in descending order

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58
papers

2,168
citations

218677

26
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223800

46
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61
all docs

61
docs citations

61
times ranked

2841
citing authors

#	ARTICLE	IF	CITATIONS
1	Origin of the Structural Phase Transition in $\text{Li}_{1-x}\text{O}_{12}$. Physical Review Letters, 2012, 109, 205702.	6.7	191
2	Tailoring Native Defects in LiFePO_4 : Insights from First-Principles Calculations. Chemistry of Materials, 2011, 23, 3003-3013.	6.7	155
3	Ab Initio Study of Deep Defect States in Narrow Band-Gap Semiconductors: Group III Impurities in PbTe. Physical Review Letters, 2006, 96, 056403.	7.8	125
4	Ab initio studies of the electronic structure of defects in PbTe. Physical Review B, 2006, 74, .	3.2	123
5	Atomic Ordering and Gap Formation in Ag-Sb-Based Ternary Chalcogenides. Physical Review Letters, 2007, 99, 156403.	7.8	123
6	Defect chemistry in layered transition-metal oxides from screened hybrid density functional calculations. Journal of Materials Chemistry A, 2014, 2, 5224-5235.	10.3	96
7	Impurity clustering and impurity-induced bands in PbTe-, SnTe-, and GeTe-based bulk thermoelectrics. Physical Review B, 2010, 81, .	3.2	86
8	Defect Physics and Chemistry in Layered Mixed Transition Metal Oxide Cathode Materials: (Ni,Co,Mn) vs (Ni,Co,Al). Chemistry of Materials, 2016, 28, 1325-1334.	6.7	78
9	Hole polaron formation and migration in olivine phosphate materials. Physical Review B, 2012, 85, .	3.2	77
10	Substitution of Bi for Sb and its Role in the Thermoelectric Properties and Nanostructuring in $\text{Ag}_{1-x}\text{Pb}_{18}\text{MTe}_{20}$ (M = Bi, Sb) ($x = 0, 0.14, 0.3$). Chemistry of Materials, 2008, 20, 3512-3520.	6.7	76
11	First-principles study of the electronic, optical, and lattice vibrational properties of AgSbTe_2 . Physical Review B, 2008, 77, .	3.2	75
12	Understanding the electronic and ionic conduction and lithium over-stoichiometry in LiMn_2O_4 spinel. Journal of Materials Chemistry A, 2014, 2, 18271-18280.	10.3	68
13	Electronic structure of Ga-, In-, and Tl-doped PbTe: A supercell study of the impurity bands. Physical Review B, 2008, 78, .	3.2	62
14	Theoretical study of deep-defect states in bulk PbTe and in thin films. Physical Review B, 2007, 76, .	3.2	57
15	First-principles studies of the effects of impurities on the ionic and electronic conduction in LiFePO_4 . Journal of Power Sources, 2012, 206, 274-281.	7.8	56
16	Defect Physics, Delithiation Mechanism, and Electronic and Ionic Conduction in Layered Lithium Manganese Oxide Cathode Materials. Physical Review Applied, 2015, 3, .	3.8	56
17	First-principles study of the formation and migration of native defects in NaAlH_4 . Physical Review B, 2009, 80, .	3.2	54
18	$\text{Na}_2\text{Fe}(\text{C}_2\text{O}_4)_2\text{F}_2$: A New Iron-Based Polyoxyanion Cathode for Li/Na Ion Batteries. Chemistry of Materials, 2017, 29, 2167-2172.	6.7	40

#	ARTICLE	IF	CITATIONS
19	Hydrogen-related defects and the role of metal additives in the kinetics of complex hydrides: A first-principles study. <i>Physical Review B</i> , 2009, 80, .	3.2	35
20	Electronic structure, polaron formation, and functional properties in transition-metal tungstates. <i>RSC Advances</i> , 2018, 8, 4191-4196.	3.6	33
21	Mechanism for the decomposition of lithium borohydride. <i>International Journal of Hydrogen Energy</i> , 2012, 37, 5825-5832.	7.1	32
22	Charge ordering and self-assembled nanostructures in a fcc Coulomb lattice gas. <i>Physical Review B</i> , 2005, 72, .	3.2	29
23	Deep defect states in narrow band-gap semiconductors. <i>Physica B: Condensed Matter</i> , 2007, 401-402, 291-295.	2.7	29
24	Defect physics in complex energy materials. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 293001.	1.8	29
25	Atomic and electronic structures of thallium-based III-V-VI ₂ ternary chalcogenides: Ab initio calculations. <i>Physical Review B</i> , 2008, 77, .	3.2	27
26	Mechanisms for the decomposition and dehydrogenation of Li amide/imide. <i>Physical Review B</i> , 2012, 85, .	3.2	27
27	Defect energy levels and persistent luminescence in Cu-doped ZnS. <i>Computational Materials Science</i> , 2019, 163, 63-67.	3.0	25
28	REAu ₂ In ₄ (RE = La, Ce, Pr, Nd): Polyindides from Liquid Indium. <i>Inorganic Chemistry</i> , 2007, 46, 6933-6941.	4.0	24
29	Reinvestigation of Na ₂ Fe ₂ (C ₂ O ₄) ₃ ·2H ₂ O: An Iron-Based Positive Electrode for Secondary Batteries. <i>Chemistry of Materials</i> , 2017, 29, 9095-9101.	6.7	21
30	Polaron formation, native defects, and electronic conduction in metal tungstates. <i>Physical Review Materials</i> , 2017, 1, .	2.4	21
31	Doping Li-rich cathode material $\text{Li}_{2-x}\text{M}_x\text{O}_4$: Interplay between lattice site preference, electronic structure, and delithiation mechanism. <i>Physical Review Materials</i> , 2017, 1, .	2.4	21
32	The Particle Size Dependence of the Activation Energy for Decomposition of Lithium Amide. <i>Angewandte Chemie - International Edition</i> , 2011, 50, 10170-10173.	13.8	19
33	Decomposition mechanism and the effects of metal additives on the kinetics of lithium alanate. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2840.	2.8	19
34	Atomic and electronic structures of I-V-VI ₂ ternary chalcogenides. <i>Journal of Science: Advanced Materials and Devices</i> , 2016, 1, 51-56.	3.1	19
35	First-principles theory of doping in layered oxide electrode materials. <i>Physical Review Materials</i> , 2017, 1, .	2.4	18
36	Hybrid density functional study of optically active Er ³⁺ centers in GaN. <i>Physica Status Solidi - Rapid Research Letters</i> , 2015, 9, 722-725.	2.4	14

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37	Role of K/Bi disorder in the electronic structure of KBi_2Te_4 . Physical Review B, 2009, 80, .	3.2	12
38	First-principles identification of defect levels in Er-doped GaN. Physica Status Solidi - Rapid Research Letters, 2016, 10, 915-918.	2.4	11
39	Tuning the valence and concentration of europium and luminescence centers in GaN through co-doping and defect association. Physical Review Materials, 2021, 5, .	2.4	11
40	Electronic Structure and Properties of Lithium-Rich Complex Oxides. ACS Applied Electronic Materials, 2019, 1, 75-81.	4.3	10
41	Magnetic Exchange in Mn^{II} [TCNE] (TCNE = Tetracyanoethylene) Molecule-Based Magnets with Two- and Three-Dimensional Magnetic Networks. Journal of Physical Chemistry C, 2015, 119, 25036-25046.	3.1	8
42	LiH as a Li^+ and $\text{H}^{\delta-}$ ion provider. Solid State Ionics, 2013, 253, 53-56.	2.7	7
43	Ionic to Electronic Transport in $\text{Ba}_3\text{Ti}_3\text{O}_6(\text{BO}_3)_2$ under Reducing Atmosphere. ACS Applied Energy Materials, 2018, 1, 510-521.	5.1	7
44	First-principles free energy calculations of the structural phase transition in LiBH_4 with I, Cl, Na, and K substitution. Physical Review B, 2013, 88, .	3.2	6
45	The role of native defects in the transport of charge and mass and the decomposition of $\text{Li}_4\text{BN}_3\text{H}_{10}$. Physical Chemistry Chemical Physics, 2014, 16, 25314-25320.	2.8	6
46	Oxygen Ion Transport and Effects of Doping in $\text{Ba}_3\text{Ti}_3\text{O}_6(\text{BO}_3)_2$. Chemistry of Materials, 2017, 29, 6425-6433.	6.7	6
47	Rare-earth defects in GaN: A systematic investigation of the lanthanide series. Physical Review Materials, 2022, 6, .	2.4	6
48	Stabilities and defect-mediated lithium-ion conduction in a ground state cubic Li_3N structure. Physical Chemistry Chemical Physics, 2016, 18, 4185-4190.	2.8	5
49	Why is it so difficult to realize Dy^{4+} in synthesized BaZrO_3 ?. Journal of the American Ceramic Society, 2022, 105, 4242-4249.	3.8	4
50	Clusters. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 37-70.	0.6	3
51	Tight-binding studies of bulk properties and hydrogen vacancies in KBH_4 . Computational Materials Science, 2013, 79, 888-895.	3.0	3
52	Rare-earth defects and defect-related luminescence in ZnS. Journal of Applied Physics, 2022, 131, 015705.	2.5	3
53	Publisher's Note: Impurity clustering and impurity-induced bands in PbTe -, SnTe -, and GeTe -based bulk thermoelectrics [Phys. Rev. B 81 , 115106 (2010)]. Physical Review B, 2010, 81, .	3.2	2
54	Formation of Small Hole Polarons in Olivine Phosphate Cathode Materials. ECS Transactions, 2012, 41, 35-42.	0.5	2

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55	Electronic Structure of AgPbmSbTem+2 Compounds – Implications on Thermoelectric Properties. Materials Research Society Symposia Proceedings, 2005, 886, 1.	0.1	1
56	Defect Clustering and Nanostructure Formation in PbTe-based Bulk Thermoelectrics. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	0
57	Atomic Ordering, Electronic Structure, and Transport Properties of LAST-m Systems. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	0
58	Electronic structure of some complex thermoelectrics – role of dimensional confinement and nanostructuring. Proceedings of SPIE, 2016, , .	0.8	0