Khang Hoang

List of Publications by Year
in descending order

58 papers	2,168 citations	218677 26 h-index	223800 46 g-index
61 all docs	61 docs citations	61 times ranked	2841 citing authors

#	Article	IF	Citations
1	Rare-earth defects and defect-related luminescence in ZnS. Journal of Applied Physics, 2022, 131, 015705.	2.5	3
2	Why is it so difficult to realize Dy⁴⁺ in asâ€synthesized BaZrO₃?. Journal of the American Ceramic Society, 2022, 105, 4242-4249.	3.8	4
3	Rare-earth defects in GaN: A systematic investigation of the lanthanide series. Physical Review Materials, 2022, 6, .	2.4	6
4	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
5	Defect energy levels and persistent luminescence in Cu-doped ZnS. Computational Materials Science, 2019, 163, 63-67.	3.0	25
6	Electronic Structure and Properties of Lithium-Rich Complex Oxides. ACS Applied Electronic Materials, 2019, 1, 75-81.	4.3	10
7	Ionic to Electronic Transport in Ba₃Ti₃O₆(BO₃)₂ under Reducing Atmosphere. ACS Applied Energy Materials, 2018, 1, 510-521.	5.1	7
8	Electronic structure, polaron formation, and functional properties in transition-metal tungstates. RSC Advances, 2018, 8, 4191-4196.	3.6	33
9	Defect physics in complex energy materials. Journal of Physics Condensed Matter, 2018, 30, 293001.	1.8	29
10	Na₂Fe(C₂O₄)F₂: A New Iron-Based Polyoxyanion Cathode for Li/Na Ion Batteries. Chemistry of Materials, 2017, 29, 2167-2172.	6.7	40
11	Reinvestigation of Na₂Fe₂(C₂O₄)₃Â·2H₂O: An Iron-Based Positive Electrode for Secondary Batteries. Chemistry of Materials, 2017, 29, 9095-9101.	6.7	21
12	Oxygen Ion Transport and Effects of Doping in Ba₃Ti₃O₆(BO₃)₂. Chemistry of Materials, 2017, 29, 6425-6433.	6.7	6
13	Polaron formation, native defects, and electronic conduction in metal tungstates. Physical Review Materials, 2017, 1, .	2.4	21
14	First-principles theory of doping in layered oxide electrode materials. Physical Review Materials, 2017, 1, .	2.4	18
15	Doping Li-rich cathode material <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> : Interplay between lattice site preference, electronic structure, and delithiation mechanism. Physical Review Materials, 2017, 1, .	2.4	21
16	Electronic structure of some complex thermoelectrics â€“ role of dimensional confinement and nanostructuring. Proceedings of SPIE, 2016, , .	0.8	0
17	Firstâ€principles identification of defect levels in Erâ€doped GaN. Physica Status Solidi - Rapid Research Letters, 2016, 10, 915-918.	2.4	11
18	Atomic and electronic structures of I-V-VI2 ternary chalcogenides. Journal of Science: Advanced Materials and Devices, 2016, 1, 51-56.	3.1	19

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19	Stabilities and defect-mediated lithium-ion conduction in a ground state cubic Li₃N structure. Physical Chemistry Chemical Physics, 2016, 18, 4185-4190.	2.8	5
20	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
21	Defect Physics, Delithiation Mechanism, and Electronic and Ionic Conduction in Layered Lithium Manganese Oxide Cathode Materials. Physical Review Applied, 2015, 3, .	3.8	56
22	Hybrid density functional study of optically active Er³⁺ centers in GaN. Physica Status Solidi - Rapid Research Letters, 2015, 9, 722-725.	2.4	14
23	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
24	The role of native defects in the transport of charge and mass and the decomposition of Li₄BN₃H₁₀. Physical Chemistry Chemical Physics, 2014, 16, 25314-25320.	2.8	6
25	Understanding the electronic and ionic conduction and lithium over-stoichiometry in LiMn₂O₄ spinel. Journal of Materials Chemistry A, 2014, 2, 18271-18280.	10.3	68
26	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
27	First-principles free energy calculations of the structural phase transition in LiBH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>with I, Cl, Na, and K substitution. Physical Review B, 2013, 88, .	3.2	6
28	LiH as a Li+ and Hâˆ’ ion provider. Solid State Ionics, 2013, 253, 53-56.	2.7	7
29	Tight-binding studies of bulk properties and hydrogen vacancies in KBH4. Computational Materials Science, 2013, 79, 888-895.	3.0	3
30	Formation of Small Hole Polarons in Olivine Phosphate Cathode Materials. ECS Transactions, 2012, 41, 35-42.	0.5	2
31	Origin of the Structural Phase Transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Li</mml:mi><mml:mn>7</mml:mn></mml:msub><mml:msub><mml:mi>La</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 109, 205702.	7.8	191
32	Decomposition mechanism and the effects of metal additives on the kinetics of lithium alanate. Physical Chemistry Chemical Physics, 2012, 14, 2840.	2.8	19
33	Mechanisms for the decomposition and dehydrogenation of Li amide/imide. Physical Review B, 2012, 85, .	3.2	27
34	Hole polaron formation and migration in olivine phosphate materials. Physical Review B, 2012, 85, .	3.2	77
35	Mechanism for the decomposition of lithium borohydride. International Journal of Hydrogen Energy, 2012, 37, 5825-5832.	7.1	32
36	First-principles studies of the effects of impurities on the ionic and electronic conduction in LiFePO4. Journal of Power Sources, 2012, 206, 274-281.	7.8	56

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37	Tailoring Native Defects in LiFePO₄: Insights from First-Principles Calculations. Chemistry of Materials, 2011, 23, 3003-3013.	6.7	155
38	The Particleâ€Size Dependence of the Activation Energy for Decomposition of Lithium Amide. Angewandte Chemie - International Edition, 2011, 50, 10170-10173.	13.8	19
39	Publisher's Note: Impurity clustering and impurity-induced bands in PbTe-, SnTe-, and GeTe-based bulk thermoelectrics [Phys. Rev. B81, 115106 (2010)]. Physical Review B, 2010, 81, .	3.2	2
40	Impurity clustering and impurity-induced bands in PbTe-, SnTe-, and GeTe-based bulk thermoelectrics. Physical Review B, 2010, 81, .	3.2	86
41	Clusters. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 37-70.	0.6	3
42	First-principles study of the formation and migration of native defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>NaAlH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:r Physical Review B, 2009, 80, .	3.2	54
43	Role of K/Bi disorder in the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î²</mml:mi><mml:msub><mml:mrow><mml:mtext>-K</mml:mtext></mml:mrow><mml:mn>2< Physical Review B, 2009, 80, .	3.2	12
44	Hydrogen-related defects and the role of metal additives in the kinetics of complex hydrides: A first-principles study. Physical Review B, 2009, 80, .	3.2	35
45	First-principles study of the electronic, optical, and lattice vibrational properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>AgSbTe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml Physical Review B, 2008, 77, .	3.2	75
46	Substitution of Bi for Sb and its Role in the Thermoelectric Properties and Nanostructuring in Ag_{1â^'x}Pb₁₈MTe₂₀ (M = Bi, Sb) (x = 0, 0.14, 0.3). Chemistry of Materials, 2008, 20, 3512-3520.	6.7	76
47	Atomic and electronic structures of thallium-basedIII-V-VI2ternary chalcogenides:Ab initiocalculations. Physical Review B, 2008, 77, .	3.2	27
48	Electronic structure of Ga-, In-, and Tl-doped PbTe: A supercell study of the impurity bands. Physical Review B, 2008, 78, .	3.2	62
49	Theoretical study of deep-defect states in bulk PbTe and in thin films. Physical Review B, 2007, 76, .	3.2	57
50	Defect Clustering and Nanostructure Formation in PbTe-based Bulk Thermoelectrics. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	0
51	Atomic Ordering, Electronic Structure, and Transport Properties of LAST-m Systems. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	0
52	REAu₂In₄ (RE = La, Ce, Pr, Nd):â€‰ Polyindides from Liquid Indium. Inorganic Chemistry, 2007, 46, 6933-6941.	4.0	24
53	Atomic Ordering and Gap Formation in Ag-Sb-Based Ternary Chalcogenides. Physical Review Letters, 2007, 99, 156403.	7.8	123
54	Deep defect states in narrow band-gap semiconductors. Physica B: Condensed Matter, 2007, 401-402, 291-295.	2.7	29

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55	Ab initiostudies of the electronic structure of defects in PbTe. Physical Review B, 2006, 74, .	3.2	123
56	AbÂInitioStudy of Deep Defect States in Narrow Band-Gap Semiconductors: Group III Impurities in PbTe. Physical Review Letters, 2006, 96, 056403.	7.8	125
57	Electronic Structure of AgPbmSbTem+2 Compounds â€“ Implications on Thermoelectric Properties. Materials Research Society Symposia Proceedings, 2005, 886, 1.	0.1	1
58	Charge ordering and self-assembled nanostructures in a fcc Coulomb lattice gas. Physical Review B, 2005, 72, .	3.2	29