Yu-Ning Wu

List of Publications by Year
in descending order

33 papers	551 citations	623574 14 h-index	642610 23 g-index
33 all docs	33 docs citations	33 times ranked	854 citing authors

#	Article	IF	Citations
1	First-principles identification of V_IÂ+ÂCu_i defect cluster in cuprous iodide: origin of red light photoluminescence. Nanotechnology, 2022, 33, 195203.	1.3	7
2	Formation of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Bi</mml:mi><mml:mstyle displaystyle="false" scriptlevel="0"><mml:mtext>â^'</mml:mtext></mml:mstyle><mml:mi>Bi</mml:mi></mml:math> Dimers in Heavily <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Bi</mml:mi></mml:math> -Doped Lead Halide Perovskites: Origin of Carrier Density Saturation. Physical Review Applied, 2022, 17, .	1.5	1
3	Temperature effect on charge-state transition levels of defects in semiconductors. Physical Review B, 2022, 105, .	1.1	7
4	MGa₂B₂O₇:Bi³⁺,Al³⁺ (M = Sr, Ba) blue phosphors with a quantum yield of 99% and negative thermal quenching. Inorganic Chemistry Frontiers, 2021, 8, 4257-4266.	3.0	7
5	Defects and dopants in zinc-blende aluminum arsenide: a first-principles study. New Journal of Physics, 2021, 23, 013018.	1.2	1
6	Defect Physics of Ternary Semiconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Zn</mml:mi><mml:mi>Ge</mml:mi><mml:mi mathvariant="normal">P</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> with a High Density of Anion-Cation Antisites: A First-Principles Study. Physical Review Applied, 2021, 15, .	1.5	15
7	Absolute Volume Deformation Potentials of Inorganic ABX₃ Halide Perovskites: The Chemical Trends. Advanced Theory and Simulations, 2021, 4, 2100060.	1.3	11
8	First-principles identification of deep energy levels of sulfur impurities in silicon and their carrier capture cross sections. Journal Physics D: Applied Physics, 2021, 54, 335103.	1.3	3
9	Intrinsic Defect Limit to the Growth of Orthorhombic HfO₂ and (Hf,Zr)O₂ with Strong Ferroelectricity: Firstâ€Principles Insights. Advanced Functional Materials, 2021, 31, 2104913.	7.8	39
10	Bandgap Engineering through Halide Doubleâ€Perovskite Alloys: A Highâ€Throughput Firstâ€Principles Study. Physica Status Solidi - Rapid Research Letters, 2021, 15, 2100343.	1.2	2
11	Energy-dependent knock-on damage of organicâ€“inorganic hybrid perovskites under electron beam irradiation: First-principles insights. Applied Physics Letters, 2021, 119, .	1.5	10
12	Enhancing neutron radiation resistance of silicon-based semiconductor devices through isotope separation and enrichment. Radiation Effects and Defects in Solids, 2021, 176, 419-430.	0.4	2
13	Temperature-dependent electronic structure of Î³-phase CuI: first-principles insights. Journal of Physics Condensed Matter, 2021, , .	0.7	0
14	First-principles exploration of oxygen vacancy impact on electronic and optical properties of ABO_{3âˆ'Î´} (A = La, Sr; B = Cr, Mn) perovskites. Physical Chemistry Chemical Physics, 2020, 22, 27163-27172.	1.3	28
15	Theoretical and experimental study of temperature effect on electronic and optical properties of TiO₂: Comparing rutile and anatase. Journal of Physics Condensed Matter, 2020, 32, 405705.	0.7	5
16	Anharmonicity Explains Temperature Renormalization Effects of the Band Gap in SrTiO₃. Journal of Physical Chemistry Letters, 2020, 11, 2518-2523.	2.1	30
17	Halide Doubleâ€Perovskite Lightâ€Emitting Centers Embedded in Latticeâ€Matched and Coherent Crystalline Matrix. Advanced Functional Materials, 2020, 30, 2000653.	7.8	30
18	NaSbSe2 as a promising light-absorber semiconductor in solar cells: First-principles insights. APL Materials, 2019, 7, 081122.	2.2	11

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19	Wu, Zhang, and Pantelides Reply:. Physical Review Letters, 2018, 120, 039604.	2.9	2
20	First-Principles Investigations of the Temperature Dependence of Electronic Structure and Optical Properties of Rutile TiO₂. Journal of Physical Chemistry C, 2018, 122, 22642-22649.	1.5	18
21	High carrier mobility in monolayer CVD-grown MoS₂ through phonon suppression. Nanoscale, 2018, 10, 15071-15077.	2.8	74
22	Fundamental Resolution of Difficulties in the Theory of Charged Point Defects in Semiconductors. Physical Review Letters, 2017, 119, 105501.	2.9	25
23	First-principles calculations reveal controlling principles for carrier mobilities in semiconductors. Semiconductor Science and Technology, 2016, 31, 115016.	1.0	8
24	Unified interatomic potential and energy barrier distributions for amorphous oxides. Journal of Chemical Physics, 2013, 139, 154506.	1.2	35
25	Giant Molecular Magnetocapacitance. Physical Review Letters, 2013, 110, 217205.	2.9	15
26	Adsorption of tris(8-hydroxyquinoline)aluminum molecules on cobalt surfaces. Physical Review B, 2012, 85, .	1.1	19
27	Adsorption of small molecules on silver clusters. Journal of Chemical Physics, 2012, 136, 024314.	1.2	25
28	Enhancement of Ag cluster mobility on Ag surfaces by chloridation. Journal of Chemical Physics, 2012, 137, 184705.	1.2	3
29	First-principles studies of Ta<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>5</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> polymorphs.	1.1	57
30	OPAL: A multiscale multicenter simulation package based on MPIâ€2 protocol. International Journal of Quantum Chemistry, 2011, 111, 4020-4029.	1.0	13
31	First-principles calculations of Fe-doped monolayer C60 on h-BN/Ni(111) surface. Journal of Chemical Physics, 2010, 132, 074702.	1.2	3
32	Accurate projected augmented wave datasets for BaFe₂As₂. New Journal of Physics, 2010, 12, 123029.	1.2	3
33	Two bonding configurations for individually adsorbed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>C</mml:mtext><mml:mrow><mml:mn>60</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> on Au(111). Physical Review B, 2010, 82, .	1.1	42