Diwen Liu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1494739/publications.pdf

Version: 2024-02-01

32 papers	501 citations	758635 12 h-index	676716 22 g-index
32 all docs	32 docs citations	32 times ranked	463 citing authors

#	Article	IF	Citations
1	A DFT study of the stability and optoelectronic properties of all-inorganic lead-free halide perovskites. Journal of Physics and Chemistry of Solids, 2022, 161, 110413.	1.9	11
2	The effect of the A-site cation on the stability and physical properties of vacancy-ordered double perovskites A2PtI6 (A = Tl, K, Rb, and Cs). Journal of Solid State Chemistry, 2022, 305, 122714.	1.4	5
3	First-principles study of the structural, electronic and optical properties of Zn1-Hg Se (x = 0, 0.25,) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	3
4	Bandgap engineering and optoelectronic properties of all-inorganic lead-free Pd-based double perovskites. Arabian Journal of Chemistry, 2022, 15, 103785.	2.3	5
5	First-principles study of the stability, electronic and optical properties of CdTe under hydrostatic pressure. Chemical Physics Letters, 2021, 764, 138272.	1.2	11
6	The mechanical, electronic and optical properties of BiPX4 (Xâ€¯=â€¯S, Se): a theoretical study. Materials Today Communications, 2021, 26, 102062.	0.9	0
7	(Li,Na)SbS2 as a promising solar absorber material: A theoretical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 250, 119389.	2.0	6
8	Stable and high efficiency mixed-cation lead-based halide perovskite: A theoretical study. Physica B: Condensed Matter, 2021, 610, 412938.	1.3	1
9	First-principles study of the stability, mechanical, electronic and optical properties of Cd0.75Hg0.25Se. Chemical Physics, 2021, 546, 111164.	0.9	3
10	Theoretical study of mixed-halide influence on the stability and electronic properties of CsCd(Cl/Br)3. Computational and Theoretical Chemistry, 2021, 1200, 113251.	1.1	2
11	Pressure-induced band gap tuning in Cs2TiBr6: A theoretical study. Journal of Solid State Chemistry, 2021, 300, 122244.	1.4	3
12	A promising all-inorganic double perovskite Rb2TiBr6 for photovoltaic applications: Insight from first-principles calculations. Journal of Solid State Chemistry, 2021, 303, 122473.	1.4	10
13	First-principles study of structural stability, electronic and optical properties of GA-doped MAPbI3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 226, 117638.	2.0	9
14	Electronic and Optical Properties of Organicâ€“Inorganic MASn1â^'xGexI3 Perovskites: A First-Principles Study. Journal of Cluster Science, 2020, 31, 1103-1109.	1.7	8
15	Insight into the Improved Phase Stability of CsPbI3 from First-Principles Calculations. ACS Omega, 2020, 5, 893-896.	1.6	34
16	Indirect-to-direct band gap transition and optical properties of metal alloys of Cs₂Te_{1â^'x}Ti_xI₆: a theoretical study. RSC Advances, 2020, 10, 36734-36740.	1.7	12
17	A first-principles study on the optoelectronic properties of mixed-halide double perovskites Cs₂TiI_{6â^'x}Br_x. New Journal of Chemistry, 2020, 44, 13613-13618.	1.4	29
18	The effect of organic cation doping on the stability and optoelectronic properties of Î±-CsPbI3. Journal of Solid State Chemistry, 2020, 290, 121577.	1.4	5

#	Article	IF	Citations
19	First-principles study of the structural stability, electronic and optical properties of CH3-F NH3GeI3 (xÂ=Â0, 1, 2, 3) halide perovskites. Chemical Physics Letters, 2020, 761, 138020.	1.2	1
20	A first-principle study of the structural, mechanical, electronic and optical properties of vacancy-ordered double perovskite Cs2TeX6 (XÂ=ÂCl, Br, I). Chemical Physics Letters, 2020, 754, 137538.	1.2	40
21	Mixed-Cation Mixed-Metal Halide Perovskites for Photovoltaic Applications: A Theoretical Study. ACS Omega, 2020, 5, 4347-4351.	1.6	13
22	Stable lead-free perovskite solar cells: A first-principles investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118493.	2.0	7
23	The effect of divalent europium doping on stability and electronic properties of CH₃NH₃PbI₃: a theoretical investigation. Applied Physics Express, 2020, 13, 101001.	1.1	2
24	Stable lead-free Te-based double perovskites with tunable band gaps: a first-principles study. New Journal of Chemistry, 2019, 43, 14892-14897.	1.4	32
25	First-Principles Modeling of Lead-Free Perovskites for Photovoltaic Applications. Journal of Physical Chemistry C, 2019, 123, 3795-3800.	1.5	18
26	Pressure-induced effects in the inorganic halide perovskite CsGeI₃. RSC Advances, 2019, 9, 3279-3284.	1.7	73
27	First-principles insight on the electronic and optical properties of Ge-based inorganic perovskites. Applied Physics Express, 2019, 12, 071007.	1.1	9
28	A comparative study of structural, electronic and optical properties based on metal-doped methylammonium lead halidesviafirst-principles calculations. New Journal of Chemistry, 2019, 43, 9453-9457.	1.4	6
29	Photovoltaic Performance of Lead-Less Hybrid Perovskites from Theoretical Study. Journal of Physical Chemistry C, 2019, 123, 12638-12646.	1.5	39
30	Ethylammonium as an alternative cation for efficient perovskite solar cells from first-principles calculations. RSC Advances, 2019, 9, 7356-7361.	1.7	33
31	Theoretical Study of the Reverse Water Gas Shift Reaction on Copper Modified Î²-Mo₂C(001) Surfaces. Journal of Physical Chemistry C, 2019, 123, 1235-1251.	1.5	39
32	Predicted photovoltaic performance of lead-based hybrid perovskites under the influence of a mixed-cation approach: theoretical insights. Journal of Materials Chemistry C, 2019, 7, 371-379.	2.7	32