Hybrid perovskites for photovoltaics insights from first principles

The three phases for MAGeI 3 in different temperatures play an important role in hybrid organic-inorganic perovskites solar cells. Up to now, their intrinsic nature still lacks systematic study. In this work, we established the crystal structures of MAGeI 3 (MA + = CH 3 NH 3 +) with orthorhombic, tetragonal and cubic phases.The electronic and optical properties of ...

First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics+. Zhenyu Wang abc, Alex M. Ganose bcd, Chunming Niu a and David O. Scanlon * bcd a Xi"an Jiaotong University, Center of Nanomaterials for Renewable Energy, State Key Lab of Electrical Insulation and Power Equipment, School of Electrical Engineering, 99 Yanxiang ...

Roknuzzaman, M. et al. Insight into lead-free organic-inorganic hybrid perovskites for photovoltaics and optoelectronics: A first-principles study. Org. Electron. 59, 99-106 (2018).

In layered inorganic materials lattice distortions can couple to break inversion symmetry and drive improper ferroelectricity, but in perovskites, symmetry prohibits such an effect. Here, the authors use group-theoretical analysis to provide crystal engineering design principles for improper ferroelectricity in molecular perovskites.

The two-dimensional (2D) hybrid halide perovskites have recently attracted attention due to their excellent photovoltaic performance. In comparison to their three-dimensional (3D) analogues, they show superior long-term durability and moisture tolerance. Meanwhile, their layered topology offers greater flexibility for electronic structure tuning. To date, most devices containing 2D ...

In this study, a first-principles density functional theory (DFT) calculations have been carried out to explore the structural, electronic, optical and mechanical properties of Pb-free organic-inorganic hybrid perovskites MABX 3 (MA = CH 3 NH 3, B = Sn, Ge; X = I, Br, Cl) and the results are compared with the Pb-containing perovskites MAPbX 3 ...

The material class of hybrid organic-inorganic halide perovskites has been rapidly progressed in the field of photovoltaic applications. However, this class of materials has limitations associated with its poor stability and toxicity of the lead element. Therefore, there is a strong desire to search for environmentally friendly perovskite materials without affecting the ...

Structural and Electronic Properties of Hybrid Perovskites for High-Efficiency Thin-Film Photovoltaics from First-Principles. The performance of perovskite solar cells recently ...

The methylammonium lead iodide perovskites at the core of recently proposed solar cells with exceptionally

large quantum conversion efficiency are studied by first-principles methods.

In recent years, Ge-based halide perovskite has gained increasing attention due to its potential in the development of lead-free perovskite solar cells. Here, through first-principles calculations ...

This Review summarizes advances in understanding the unique physical properties of hybrid perovskites that enable the fabrication of high-efficiency solar cells with high open ...

First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics. March 2018; ... solid-state hybrid perovskite solar cells in 2012, 4. power.

Unparalleled coverage of the most vibrant research field in photovoltaics! Hybrid perovskites, revolutionary game-changing semiconductor materials, have every favorable optoelectronic characteristic necessary for realizing high efficiency solar cells. The remarkable features of hybrid perovskite photovoltaics, such as superior material properties, easy material ...

The performance of perovskite solar cells recently exceeded 15% solar-to-electricity conversion efficiency for small-area devices. The fundamental properties of the active absorber layers, hybrid ...

Hybrid halide perovskite solar cells have recently attracted substantial attention, mainly because of their high power conversion efficiency. Among diverse variants, (CH3NH3)PbI3 and HC(NH2)2PbI3 ...

Organic-inorganic hybrid perovskites have attracted extensive attention as promising photovoltiac materials for high-efficiency solar cells. In this study, strain effects on the material properties of Ge-based perovskites are fully investigated by the first-principles calculations. The results indicate that the structural, mechanical, electronic and optical ...

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run towards efficient and economically feasible photovoltaic devices spotlights the class of MPbI 3-xCl x hybrid (i.e., mixed organic-inorganic) perovskites, where M labels the methylammonium...

Hybrid perovskites are currently one of the most active fields of research owing to their enormous potential for photovoltaics. The performance of 3D hybrid organic-inorganic ...

Although, there have been numerous studies that investigated the structural and electronic properties of the inorganic Ge-based mono halide perovskites using the First Principles Calculations [13 ...

The three phases for MAGeI3 in different temperatures play an important role in hybrid organic-inorganic

perovskites solar cells. Up to now, their intrinsic nature still lacks systematic study.

The two-dimensional (2D) hybrid halide perovskites have recently attracted attention due to their excellent photovoltaic performance. In comparison to their three-dimensional (3D) analogues, they show superior long-term durability and moisture tolerance. Meanwhile, their layered topology offers greater flexi

Generally, the structural formula of organic-inorganic hybrid halide perovskite is referred to ABX 3, where A is the organic cation MA + (MA=CH 3 NH 3) or FA + (FA=CH(NH 2) 2), B is the metal cation, and X is the halide anion. Among them, methylammonium lead iodide (MAPbI 3) has attracted significant attention for its excellent light absorption ...