

From unusual semiconductors at the atomic scale to potentially promising devices.

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ABSTRACT

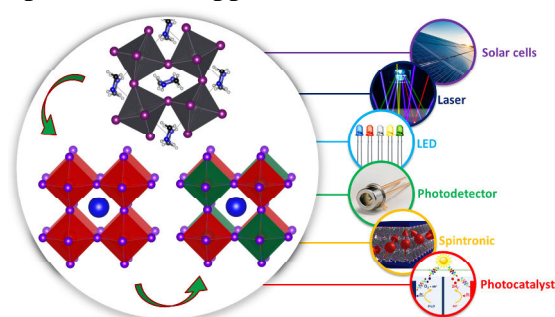
The climate change and its impacts are nowadays well established and cannot be ignored [1]. The international community agrees to have a fast energy transition, which translates in developing more efficient photovoltaic cells, light emitting and photocatalytic devices.

Halide perovskites have captivated the research community over the past 7 years mainly in the photovoltaic field. These materials have first emerged as a new generation of absorber materials for high-efficiency and low-cost solar cells [2], [3]. Indeed, unusually good optoelectronic properties for materials grown at low temperatures are associated to excellent absorbing capabilities yielding highly efficient photovoltaic devices. Nowadays, halide perovskite single junction solar cells have reached power conversion efficiency (PCE) higher than 25% [3]. Moreover, halide perovskites exhibit attractive potential for others optoelectronic applications such as Lasers, Light Emitting Devices (LEDs), Photodetectors, Photocatalysis.

Nevertheless, despite promising low manufacturing costs, short payback time and abundant material resources, the potential industrial use of halide perovskites is actively debated. Major potential concerns have been raised in the initial period about the presence of Pb atom which leads to toxicity issue, the long term materials and device stability and the device upscaling.

Researchers are also working on finding alternative materials such as perovskite-like structures [4], non-perovskite structures (rudorffites [5]) or even double perovskites [6] which may tackle simultaneously these 3 issues. Additionally, recent theoretical studies based on Density Functional Theory to predict thermodynamic, electronic and optical properties will be presented.

The *ab initio* simulations have been performed on HPC resources of CINES and TGCC under the allocation 2019-[x2019096724] made by GENCI (Grand Equipement National de Calcul Intensif).



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