Towards high-efficient and stable all-iniorganic perovskites as sun-light absorber materials

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Description:

Proyecto asignado a través de la Red Española de Supercomputación (RES [2]).

Hybrid organic-inorganic lead halide perovskites have earned much consideration for their use in photovoltaic devices, wich efficiencies as high as 23%. But yet important challenges need to be overcome: poor stability and the toxicity of Pb. This project purpose the search for suitable perovskite semiconductor materials with enhanced stability, low toxicity as well as improved sunlight conversion efficiencies. Both, the intrinsic stability (replacing the organic cations by inorganic ones) and toxicity (by reducing Pb quantity) problems of perovskite materials can be fixed by adjusting the chemical composition. Thus, the effect of the chemical composition of all-inorganic perovskites with general formula Cs1-aRbPb1-bSnbI2Br on stability and sub-light absorption related-properties by using ab-initio methods.

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