Photo-sensitization of doped ferroelectric oxides using a high-throughput framework.

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Description:

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

Perovskites have revolutionized solar cell research obtaining efficiencies up to 22% in less than 10 years. In contrast to conventional solar cells, the efficiency of this new generation of solar cells is not controlled by the Shockley-Queisser limit. Ferroelectric materials exhibit a spontaneous electric polarization facilitating the excited carrier separation which is known as bulk photovoltaic effect. While ferroelectric oxides perovskites excel separating effectively excited charges, thy are far for being good sunlight harvesters. Different strategies have been proposed to tune their electronic properties, but doping is the most common route to modify their electronic properties. In this activity, we strive to apply high-throughput techniques to tune the electronic structure of ferroelectric oxides by doping.

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Links

[1] http://www.us.es/ [2] https://www.res.es/