Cation substitution effects on the structural, electronic and sun-light absorption features of all-inorganic halide perovskites

All-inorganic perovskites (such as $CsPbI_3$) are emerging as new candidates for photovoltaic applications. Unfortunately, this class of materials present two important weaknesses in their way to commercialization: poor stability and toxicity. This paper explores the possibility of lessening both stability and toxicity related problems, as well as obtaining improved photovoltaic efficiencies through the propitious fine-tuning of the chemical composition. Therefore, a systematic *ab initio* study of the family of all-inorganic perovskites with the general formula $Rb_aCs_{1-a}Sn_bPb_{1-b}I_2Br$ (a = 0–0.125 and b = 0–1) is here presented.

Our results provide a complete description on the connections between the chemical composition, crystal structure, intrinsic stability, electronic properties, and absorption features, pointing out that all-inorganic $Rb_aCs_{1-a}Sn_bPb_{1-b}I_2Br$ (a = 0.125 and 1 > b > 0.5) perovskites would be adequate candidates for photovoltaic applications with improved stability and reduced Pb concentration.

Fuente de la publicación:

- Pablo Sánchez-Palencia, Gregorio García, Perla Wahnón & Pablo Palacios. Cation substitution effects on the structural, electronic and sun-light absorption features of all-inorganic halide perovskites. *Inorganic Chemistry Frontiers*, 2022. https://doi.org/10.1039/D1QI01553B [1]

Noticias relacionadas:

- Investigadores de la Universidad Politécnica de Madrid, publican los resultados de un importante trabajo usando recursos computacionales de CénitS [CénitS [2]].

Links
[1] https://doi.org/10.1039/D1QI01553B [2] http://www.cenits.es/noticias/31032022-investigadores-universidad-politecnica-madrid-publican-resultados-importante