

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 $\text{Rb}_a\text{Cs}_{1-a}\text{Sn}_b\text{Pb}_{1-b}\text{I}_3\text{Br}$ ($a = 0-0.125$ 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 $\text{Rb}_a\text{Cs}_{1-a}\text{Sn}_b\text{Pb}_{1-b}\text{I}_3\text{Br}$ ($a = 0.125$ 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]].

URL del envío: <https://web.computaex.es/enlaces/publicaciones/cation-substitution-effects-structural-electronic-and-sun-light-absorption>

Enlaces

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