Triphenylene-based molecules as Organic Spacers for tuning structure and electronic properties of 2D perovskites materials

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Idioma Español

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

Two-dimensional (2D) hybrid organic-inorganic perovskites have shown great application potential in solar cells and other optoelectronic devices. Based on DFT simulations and AIMD, we study the structure, stability and electronic-structure related properties of a series of 2D Ruddlesden-Popper and Dion-Jacobson perovskites, which adopt the general formula Y2BX4 and YBX4, respectively, with Y = TriPh-based organic bication or cation, B = Pb, Sn; X = Cl, Br, I).

Web:

URL del envío:https://web.computaex.es/proyectos/triphenylene-based-molecules-organic-spacers-tuning-structure-and-electronic-properties-2d

Enlaces
[1] https://www.uva.es/export/sites/uva/ [2] https://www.res.es/