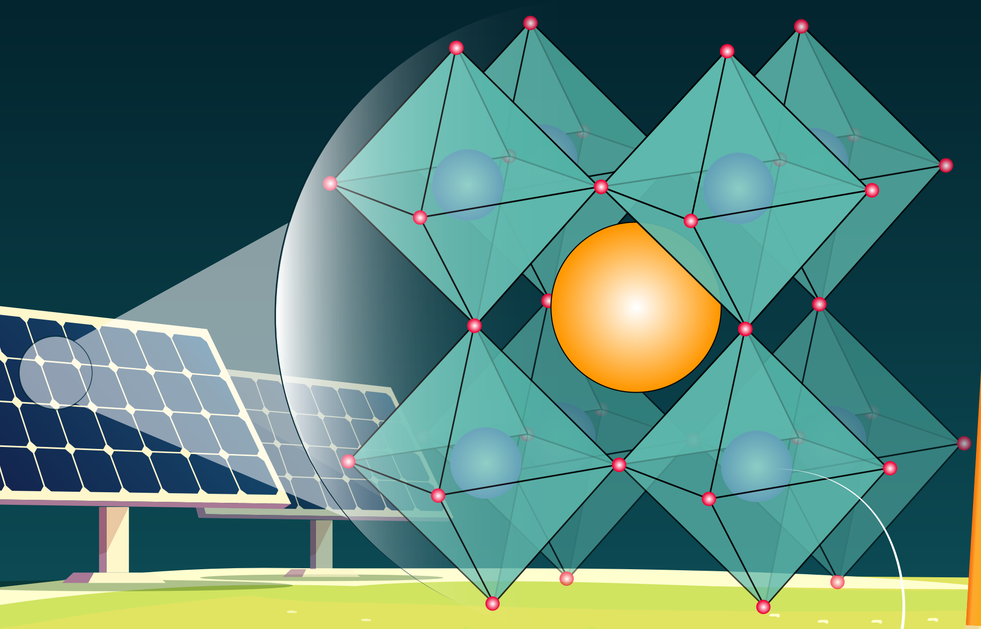
A Pencil and Paper Approach for Identifying Exciting New Halide Double Perovskites

Lead-halide 3D perovskites show promising photovoltaic performance



But, the toxic lead content makes them less desirable

Pb

Double perovskites ($A_2BB'X_6$) can be a suitable alternative, but they have complex and diverse electronic structure

A theoretical method to predict perovskites with suitable bandgaps to act as potential solar absorbers

Linear combination of atomic orbitals [LCAO]

1. Double perovskite crystal structure
2. Linear combinations of halide orbitals
3. Applying translational symmetry
4. Adding metal interactions

Input

Atomic orbitals of the B and B' metals

Modified LCAO

Output

Bandgap

This modification of the LCAO approach allows us to apply it to all halide double perovskites

The modified LCAO approach is expected to help the synthesis of new and interesting double perovskite compositions which can act as potential solar absorbers

Chemical Science

PICK OF THE WEEK

A pencil-and-paper method for elucidating halide double perovskite band structures

Slavney *et al.* (2019) | DOI: 10.1039/C9SC03219C

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