Poster

Lattice constants prediction and thermochemistry of hexahalometallate A 2 MX 6

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A_2MX_6 perovskites materials have shown impressive advances in the last 50 years due on thier photovoltaic application , made them one of the most-promising technologies for next-generation solar cells. We present in this work a semiempirical model for prediction of mail parameter of cubic A2MX6 perovskites. It is useful for providing the predicted structural information for estimating the physical properties of materials for which accurate structural data are not available.

We propose a linear formula according to the factors:

1. Interatomic distance R_A + R_X and R _M + R_X and electro negativity difference χ_X-χ_M.
2. The interatomic distances d (A-M) and d (M-M) can be estimated from the crystalline structure of the compounds studied.

A new prediction of mail parameter is estimated for 89 perovskites and the results are compared with the experimental one whose error is of the order of 2.13%.