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TÉMA

High-throughput computational design of photocatalytic materials

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The search for new photocatalytic materials is enhanced by computational materials by design algorithms. Here, we present the application of high-throughput calculations to a class of photocatalytic delafosside oxide materials. In these materials, there is an intriguing problem of a forbidden optical transition (Laporte selection rule), which is prototypical of many delafossite systems, yielding transparent, but conducting materials. Delafossite oxides are of the form ABO_2, hence alloying at the A or B site will yield an alloyed material with enhanced photo-absorption resulting from symmetry breaking. We will present results of $AB1_{1-x}B2_xO_2$ alloys using high-throughput calculations and data mining techniques, we show the most likely positional configurations for $x = 0.00$ through $x = 0.10$ of the B2-site atoms relative to one another. Implications of this result and applications of the techniques used are discussed, including the development of candidate materials via high-throughput analysis of constituent search-space. We will present the optical properties of optimal (energetically) delafossite oxide candidates.

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