

Electronic band structure of Pb-substituted layered perovskite materials

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Perovskite-type oxide materials based on transition metals with d(0) electron configuration such as Nb(V), Ta(V), and Ti(IV) are efficient photocatalysts for overall water splitting with high quantum yields. However, the band gaps of these materials (ca. 3.8–4 eV) are not adequate for visible light-induced photocatalysis. The development and fabrication of materials showing photocatalytic activity for water splitting into H₂ and O₂ and degradation of organic pollutants under visible light irradiation, therefore, is the most important topic in the photo-catalysis research today.

In the present study, band gaps of Pb-substituted layered perovskite materials were investigated using Full Potential Linerized Augmented Plane Wave (FLAPW) method.