Abstract

Photocatalysis through perovskite is becoming an emerging trend for scientists as it can be used in solar cells to consume solar energy. Solar energy is easily available, creates no pollution, and is less costly that's why researchers are taking an interest in its production. A sustainable society must be achieved by lowering greenhouse gas emissions and damage to the environment through the use of clean and renewable energy sources.

Photo-catalysis is a vital technology in addressing global issues including the energy crisis and environmental degradation by utilizing sustainable energy sources, such as solar energy. Therefore, it is crucial to design and produce photo-catalysts that are prevalent on Earth, inexpensive, and have excellent performance for water splitting and wastewater treatment. Various perovskite photo-catalysts have been created utilizing different methods and efforts, with the aim of predicting their physical and chemical stability as well as their optoelectronic capabilities. This has been achieved by theoretical and computational investigations, employing various combinations and permutations. This article provides a comprehensive examination of the various changes in structure and composition that can enhance the photocatalytic performance of perovskite photo-catalysts. In this research, we are using $SrNbO_{3-x}H_x$ with the concentration of (□ = 0.0, 0.3, 0.6 0.9, 1.2, 1.5, 1.8, 2.1, 2.4, 2.7, 3.0) for the process of Photocatalysis water splitting. This method produces the H_2 and O_2 without producing harmful gases so we can use the H_2 for the production of fuel cells and solar cells. These fuel cells will be a replacement for fossil fuels to fulfill future energy demands. Our material's stability is confirmed by the results of elastic constants and tolerance factors. Its tolerance factor is 0.8102 which confirms its structural stability. By increasing the hydrogen inclusion in $SrNbO_{3-x}H_x$ its bandgap reduces from 2.38 eV to 1.53 eV. Reduction in bandgap clarifies that this is the best material to use for the Photocatalysis water splitting method. Decrement in bandgap also affects the material's optoelectronic properties. The main objective of this paper is to provide some suggestions for the future use of materials based on perovskites in environmental cleanup.