

Photocatalytic properties and electronic structure of $\text{Ca}_2\text{Nb}_2\text{O}_7$ layered perovskite material

김현규^{1,*}, 홍태은¹, 박혁규^{1,2}, 정의덕¹, 김해진³,
지상민⁴, 배상원⁴, 홍석준⁴, 장점석⁴, 이재성⁴
¹한국기초과학지원연구원 부산센터; ²부산대학교 물리학과;
³한국기초과학지원연구원 미래융합연구실;
⁴포항공과대학교 화학공학과
(hhgkim@kbsi.re.kr*)

Among various methods of solar energy conversion, much attention has been paid to the photocatalytic water splitting for its potential significance in obtaining directly clean and high energy containing H_2 from abundant H_2O . The perovskite materials such as SrTiO_3 and CaTiO_3 have photocatalytic activities for water splitting under UV light irradiation. However, the quantum yields are very low (ca. <1%). Thus there is need to explore the photocatalytic properties of newer materials.

In this paper, we report the photocatalytic properties of highly donor-doped (110) layered perovskite material, $\text{Ca}_2\text{Nb}_2\text{O}_7$, along with its electronic band structure calculations. We further discuss the experimental and theoretical results in light of the photocatalysis. The photocatalytic and electronic properties indicate $\text{Ca}_2\text{Nb}_2\text{O}_7$ to be a better photocatalyst than conventional or other known candidates viz. TiO_2 , SrTiO_3 , BaTiO_3 .