Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Photoexcitation Mechanism of Metallic $Sr_{1-x}NbO_3$ for Water-splitting Photocatalyst MASANORI KANEKO, Univ of Tokyo, GIACOMO GIORGI, Universit degli Studi di Perugia, KOICHI YAMASHITA, Univ of Tokyo
— The absence of a bandgap makes metallic materials not suitable as water-splitting photocatalysts. In 2012, Xu et al. have reported results about Sr-vacancy $SrNbO_3$ as a water-splitting photocatalyst.[1] Surprisingly, this species is metallic (implying high carrier mobility) with an optical gap of about 1.9 eV and absorb most of the visible light. Authors, by means of DFT based calculations, have predicted its band structure and showed that three bands are separated by a gap: occupied band (B_{-1}), partially empty band (CB), and unoccupied band (B_1). More recently several studies have focused on the energy gap of this class of materials. Nevertheless, the results of the photoexcitation of $SrNbO_3$ obtained so far are controversial. Accordingly, we focused my attention on the optical absorption and the position of the bands by means of a DFT analysis. We revealed that photoexcitation around optical gap 1.9 eV is constituted by the CB$\rightarrow B_1$ transitions on some k-point along the $\Gamma - X$ direction and the most contributed k-point isn't placed in the band-diagram. In addition, we investigated the effect of Sr vacancies and substitutionals on the bandstructure and light absorption.

[1]X. Xu, et al., **Nature Materials**, 11, 595 (2012)

Masanori Kaneko
Univ of Tokyo

Date submitted: 11 Nov 2016 Electronic form version 1.4