

## The influence of oxygen vacancy on the linear and nonlinear optical properties of $\text{Pb}_7\text{O}(\text{OH})_3(\text{CO}_3)_3(\text{BO}_3)$

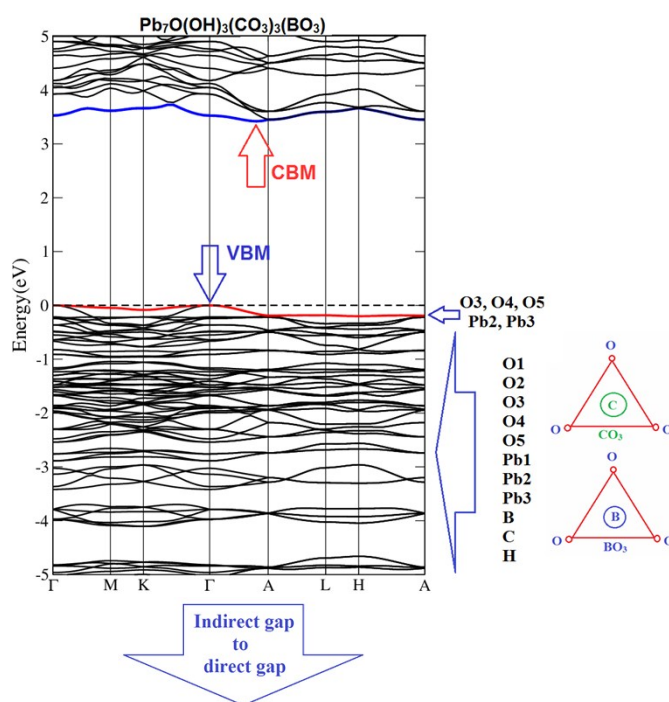
A. H. Reshak<sup>1,2,\*</sup>, S. Auluck<sup>3</sup>

<sup>1</sup>*New Technologies - Research Centre, University of West Bohemia, Univerzitni 8, 306 14  
Pilsen, Czech republic*

<sup>2</sup>*School of Material Engineering, University Malaysia Perlis, 01007 Kangar, Perlis,  
Malaysia*

<sup>3</sup>*Council of Scientific and Industrial Research - National Physical Laboratory Dr. K S  
Krishnan Marg, New Delhi 110012, India*

### Supplementary materials



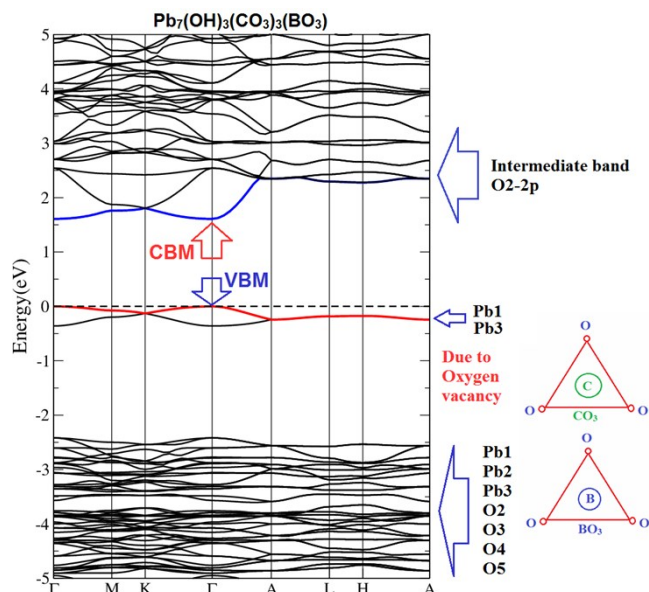


Fig. S1: Calculated electronic band structure of I and II.

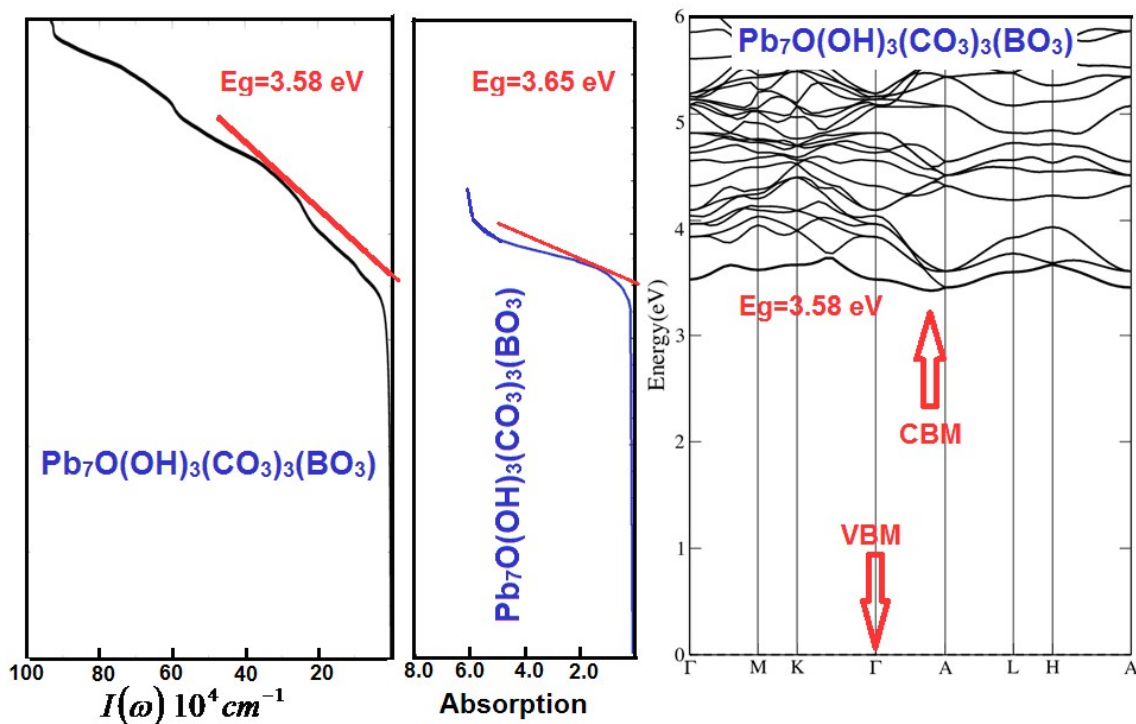


Fig. S2: The calculated absorption (shown in the first figure) is in good agreement with the extracted experimental data (shown in the second figure). The calculated energy band gap (shown in the third figure) is also in good agreement with the experiment.