Influence of Oxygen Vacancy on the Electronic Structure of the Asymmetric Mixed Borate-Carbonate Pb₇O(OH)₃(CO₃)₃(BO₃)

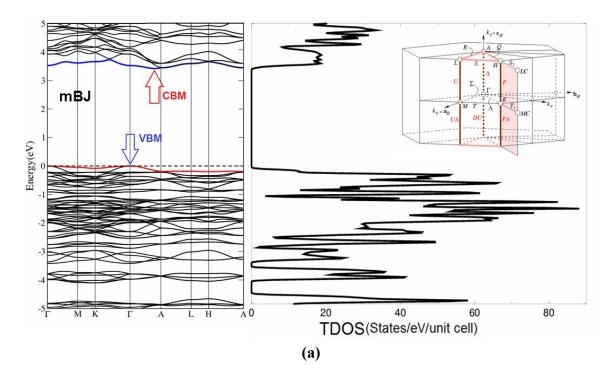
A. H. Reshak^{1,2,*}, Sushil Auluck^{3,4}

¹New Technologies - Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech republic

 ² Center of Excellence Geopolymer and Green Technology, School of Material Engineering, University Malaysia Perlis, 01007 Kangar, Perlis, Malaysia
³ Council of Scientific and Industrial Research - National Physical Laboratory Dr. K S Krishnan Marg, New Delhi 110012, India

⁴Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India

Supplementary materials



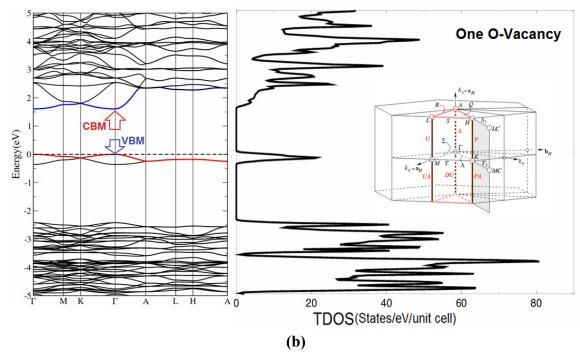


Fig. S1: The total density of states (TDOS) along with the electronic band structure and the first BZ are shown for I and II. It is clear that the oxygen vacancy significantly influences the TDOS.