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Oxygen vacancy and hole conduction in "leaky" amorphous TiO2 from first-principles calculations HIEU PHAM, LIN-WANG WANG, Lawrence Berkeley National Laboratory — In the last decade, titanium dioxide (TiO_2) has been one of the most studied materials due to its low cost, lightweight, eco-friendliness and long-term stability to be used in energy applications. Specifically, it was found recently that amorphous TiO_2 could be used as a protection layer for photo-induced water splitting. While protecting the light-absorbing photoanodes from corrosion, it can conduct hole carriers, perhaps through some defect levels. Nevertheless, the exact mechanism for such hole conductivity is not clearly understood. In this work, an amorphous TiO_2 model is obtained from molecular dynamics employing the melt-and-quench technique. The electronic properties, polaronic states and hole conduction mechanism in amorphous structure were investigated by means of density functional theory. The formation energy of oxygen vacancy was found to reduce significantly (by a few eV) upon the amorphization. Our theoretical study suggested that the oxygen vacancies and their defect states provide hopping channels which are comparable with experimental observations and could be responsible for the hole conduction in the "leaky" TiO_2 recently discovered for the photochemical water-splitting applications.

Hieu Pham
Lawrence Berkeley National Laboratory

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