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Does $\beta - PbO_2$ Harbor Topological States? SHARAD MAHATARA, BORIS KIEFER, Department of Physics, New Mexico State University, Las Cruces NM, USA — The electronic properties of $\beta - PbO_2$, have been controversial for over a century. Experiments find metallic behavior, attributed to its defect structure, to indirect semiconducting for stoichiometric samples, with a gap of 0.61 eV. Theory leads to similar ambiguities, and predicts this phase to be metallic (PBE, HSE06) or the opening of too small bandgap (HSE06). An area where this inconsistency is significant, is when a material property depends on the electronic structure in the vicinity of the Fermi energy, such as topological states. In our work, we use a self-consistent DFT+U approach and find stoichiometric $\beta - PbO_2$ to be an indirect semiconductor with a band gap of $\sim$ 0.8 eV, similar to experiment. The larger bandgap requires strains of $\sim 4\%$ to drive $\beta - PbO_2$ into a nodal line semimetallic state, which is not protected under the application of spin-orbit-coupling. These insights are also supported by our surface computations, that do not show any topologically protected states near the Fermi energy. Therefore, our results show that in contrast to previous computations $\beta - PbO_2$ is a topologically trivial material, consistent with experiment, an observation that can be attributed to the inaccurate optical properties in previous work.

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