

Abstract Submitted
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Electronic Structures of Oxygen-deficient PtO₂¹ YONG YANG, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, 305-0047, Japan, OSAMU SUGINO, 1. National Institute for Materials Science; 2. Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa 277-8581, Japan, TAKAHISA OHNO, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, 305-0047, Japan — We studied the electronic properties of beta-platinum dioxide (β -PtO₂), a catalytic material, based on density functional theory. Using the GGA+U method whose predicted band gap is verified by GW calculations, we found that the creation of an oxygen vacancy will induce local magnetic moment on the neighboring Pt and O atoms. The magnetism originates not only from the unpaired electrons that occupy the vacancy induced gap state, but also from the itinerant valence electrons. Because of antiferromagnetic (AF) coupling and the localized nature of gap states, the total magnetic moment is zero for charge-neutral state (V_{O}^0) and is $\sim 1 \mu_B$ for singly-charged states (V_{O}^{\pm}). Calculation of grand potential shows that, the three charge states ($V_{\text{O}}^0, V_{\text{O}}^{\pm}$) are of the same stability within a small region, and the negatively charged state (V_{O}^-) is energetically favored within a wide range of the band gap. On this basis we discussed the implication on catalytic behavior.

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