The origin of different iridium oxidation states of Sr2IrO4

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Abstract: The results of ab initio calculations performed for Sr2IrO4 using the density functional theory with the spin-orbit coupling and the onsite Hubbard-U correction applied to the Ir-d states are reported in order to provide more insights into known experimental data. The results demonstrate that in the stoichiometric oxide all Ir ions are in the +4 oxidation state. In the presence of an O vacancy some Ir ions turn into +3 and +2 states that is contrary to experimental observations where only the +3 state has been observed. These transitions are accompanied by the change in the magnetic moments from 0.10 ?B for Ir4+ to 0.26 ?B and 0.31 ?B for Ir3+ and Ir2+, respectively. Depending on the site where the O vacancy is formed, the change in the oxidation state leads to either the appearance of empty defect states in the gap or filled localized Ir d-states. The reasons for the absence of the Ir2+ state in experimental data are also discussed. The formation of a Sr vacancy does not cause alternation in ion oxidation states providing instead a remarkable change in the band structure of the oxide resulting in the appearance of Dirac cones at the Fermi level. No experimentally determined Ir5+ state could be detected in the presence of an Ir vacancy or an additional interstitial

oxygen indicating a more complex nature of defects to provide the +5 state.

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