Effects of bipolarons on oxidation states, and the electronic and optical properties of $W_{18}O_{49}$

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2021

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Keywords: Tungsten oxides, bipolaron formation, oxidation state, absorption coefficient, shielding effect

Abstract: $W_{18}O_{49}$ has been studied by means of ab initio techniques in the framework of the density functional theory using the onsite Hubbard-U correction applied to the W-d states as well as using the hybrid potential. The existence of bipolarons is found to be an intrinsic feature of this oxide resulting in the presence of different oxidation states of W atoms (W^{6+} and W^{5+}) and in the co-existence of localized and delocalized electrons. We also discuss possible switching from the W^{6+} to W^{5+} and from the W^{5+} to W^{4+} oxidation states in the presence of an O vacancy. It appears that O vacancy formation does not cause any additional charge localization at W sites but solely contributes to delocalized electrons. The calculated absorption and reflection

coefficients manifest a transparency window in the visible region. At the same time, sizable absorption, occurring due to the presence of free carriers, is detected in the far and mid infrared regions. Additionally, in the near infrared region we confirm and explain an experimentally observed shielding effect originating from transitions involving the localized bipolaronic states.

This article published in: Migas, D. B. Effects of bipolarons on oxidation states, and the electronic and optical properties of $W_{18}O_{49}$ / D. B. Migas, A. B. Filonov, N. V. Skorodumova // Phys. Chem. Chem. Phys. – 2021. – Vol. 23. – № 45. – P. 25824-25829. – DOI:10.1039/d1cp02634h.

Internet-link for the article:

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