Journal of Organometallic Chemistry, vol. 766, 2014, pages 22-33

Theoretical calculations for MUO3 (M = Na; K; Rb): DFT + U study

Abstract

The energy band structure, density of states and electronic charge density for MUO3 (M = Na; K; Rb) compound has been inspected in support of density functional theory (DFT). We have employed the GGA + U to treat the exchange correlation potential by solving Kohn-Sham equations. It is well known that density functional theory underestimates band gaps of materials which have highly localized valence electrons. On the other hand, the predictions of electronic properties of materials, which do not have localized band near the band gap, by DFT are not accurate enough as well. The effect of electronic correlation on properties of MUO3 (M = Na; K; Rb) compound is theoretically studied in this paper. The calculations show that the investigated compounds are semiconductor with direct/indirect energy gap of about 4.466, 4.652 and 4.326 eV for NaUO3 KUO3 and RbUO3, respectively. The density of states expresses that valence band is mostly dominated by U-s/p/f and O-p states. While the conduction band is composed of U-f/d and Na/K/Rb-s/p orbitals. Covalent bond is formed between U and O atoms as can be seen from PDOS that U-p and O-d states hybridized around -0.2. The linear optical properties were also discussed in particular.

Keywords

Electronic charge density; Electronic structure