Using design principles to systematically plan the synthesis of hole-conducting transparent oxides: Cu_3VO_4 and Ag_3VO_4 as a case study

T m , J m, J. m
020 ,
V m , m
020 ,
*
0 0 ,
0 0 ,

(2 2011, m 12 J 2011, 14 2011)

f (T), m f m f f ( ) m m f T f m f 2 2 f m f m f m f V 3 4 V 3 4, V .

4 ff m , 3V 4 (= 0.1), m f , f m f T T f - V 3 4 2. V , m m m f 2.1V , f .

10.1103/ ./ 4.1 11 m ( ), 1.20 , 1. , 4. 2. , 1. .

I. DESIGN PRINCIPLES OF *p*-TYPE TRANSPARENT CONDUCTING OXIDES

(T) f m f f m [1] T m m J m m f m (m) - m m V( ). m - T m f ( )[2] f ( ) (.,) f m , m m f m (m m f) m - f) m . ( ) - (.,), f f m [4] T m m [3] V m f , m , f

II. ASSESSMENT OF THE BASELINE *p*-TYPE BINARY OXIDES Cu_2O AND Ag_2O AGAINST THE DPs

A. Thermodynamic stability of the host binaries

m m (Δ) f m

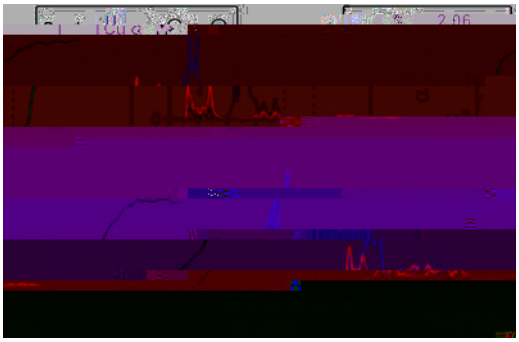
m f f

$$\Delta + \Delta = \Delta ( ), \quad (1)$$

$$\Delta \leqslant 0, \quad \Delta \leqslant 0, \quad (1)$$

$$'\Delta + '\Delta \leqslant \Delta ( ). \quad (1)$$

T m f ff Δ m ° f f f (1) f m m - m f m f m Δ ( ) f f m f f f m (1) f m Δ m f f m (1), f m m ff m m m , f f m f m m f m f m f m f m f , . (1) m f m , m Δ 2 f m f m f m f f m f m f m , m f m 2, f f m , f f m . T ff f m f m + m f f f + m f m 2( ) 2( )



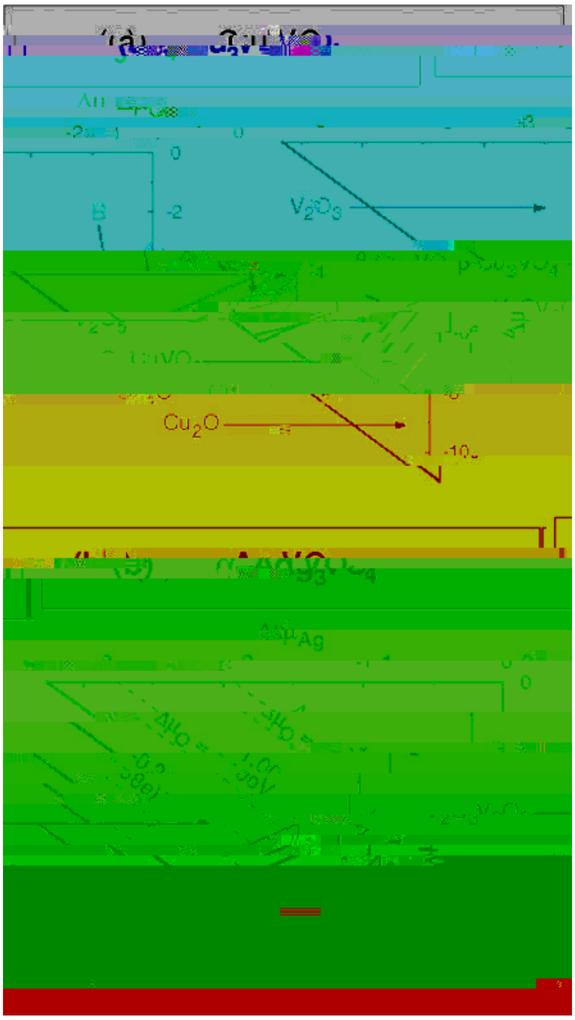
. 4. ( ) f (f- -
) m ( ) f
m
( ) ( ) -m
. T f
V
f
( ).

V
m m , m
f m 2 f m f m
f m f f m 2 2 .

C. Band-structure properties of Cu_2O and Ag_2O: Optical properties of the binaries

4
f m f
(f 21) m (f
f f).
2 2 f
m f
ff T f -m
m f ,
f - m m m. T -

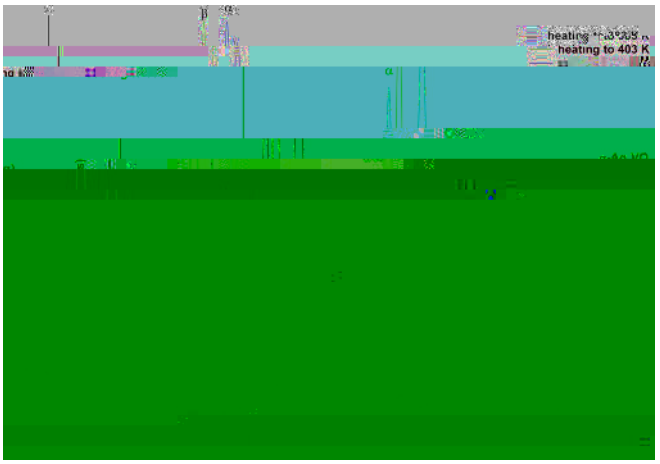
C. Crystal structures of Ag_3VO_4 and Cu_3VO_4



[illegible]

0 −1.01V

[illegible]



. / . ( ) m f V 3 4.

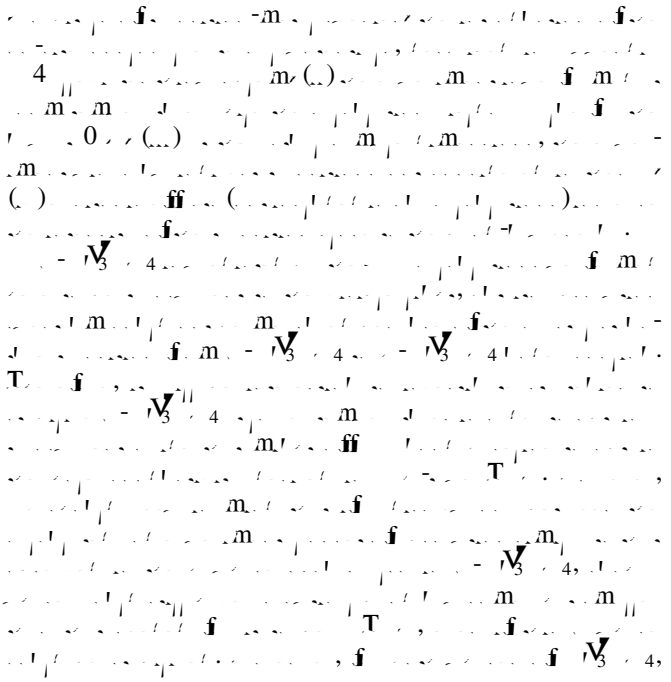
m , - V 3 4 f m f - V 3 4 , - m - ff m ( ), / , f m , - V 3 4 - V 3 4, 3/ 3 , f m 403 f m - V 3 4 m , 333 , - V 3 4 f m - V 3 4 . T m [2/] T f - V 3 4 330 m 2 / m - V 3 4. T m f V 3 4 [31]

B. Intrinsic defects, hole generation, and hole density in Cu_3VO_4 and Ag_3VO_4

( ) ( )

m f f f m m f m m m f f f ( ) f m , m f ff m [32,33] *

(



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