84, 1 11 (2011)

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

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(T), $_2$ $_2$ $_3$ $_4$ $_3$ $_4$,

$_4$ $_3$V $_4$ (= 0.1), T T V $_4$ 2. V , 2.1V ,

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( ) 1.20 1. 4. 2. 1.

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

(T) [1] T ( ) V ( ). T ( )[2]

(.) ( ) ( ) ( )

(..) ( ), [3] T V

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

A. Thermodynamic stability of the host binaries

[illegible] (Δ) [illegible]

$$\Delta \; + \; \Delta \; = \Delta \; (\;), \qquad (1\;)$$

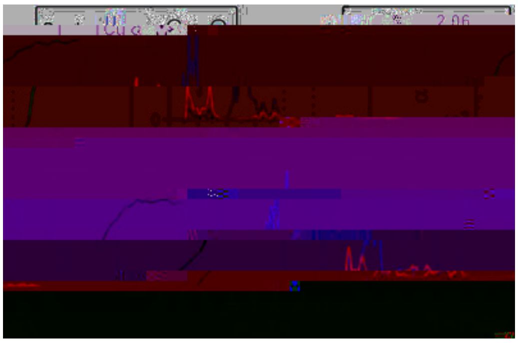
$$\Delta \; \leqslant 0, \quad \Delta \; \leqslant 0, \qquad (1\;)$$

$$'\Delta \; + \; '\Delta \; \leqslant \Delta \; (\;). \qquad (1\;)$$

T [illegible] Δ [illegible] (1) [illegible] Δ ( ) [illegible] (1) [illegible] Δ [illegible] (1), [illegible] (1) [illegible] Δ [illegible] 2 [illegible] 2, [illegible] T [illegible] + [illegible] + [illegible]

[illegible] 2( ) [illegible] 2( )

[illegible]



[illegible] 4. [illegible]

[illegible]

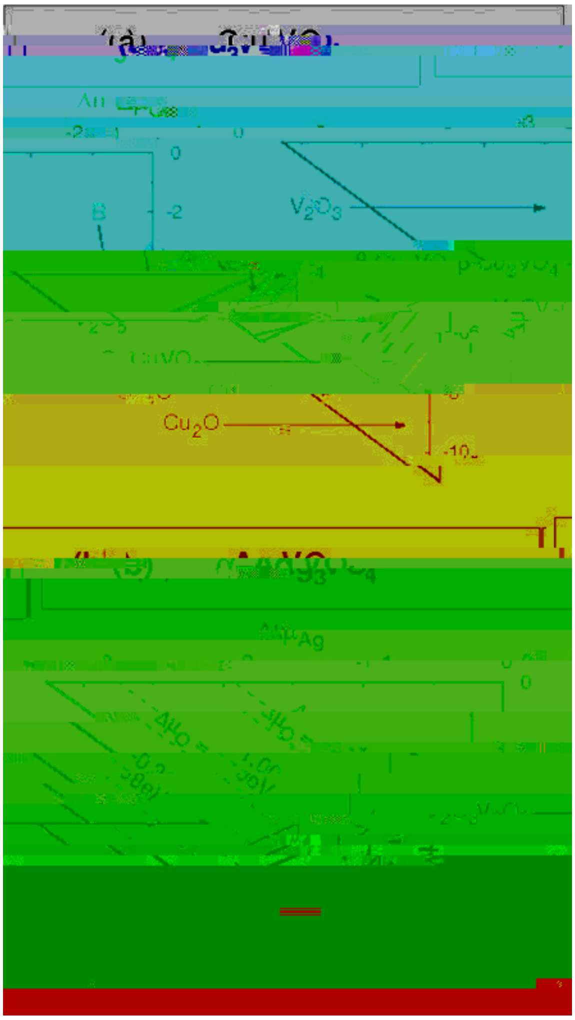
[illegible]

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

[illegible] 4 [illegible] 21) [illegible]

[illegible]

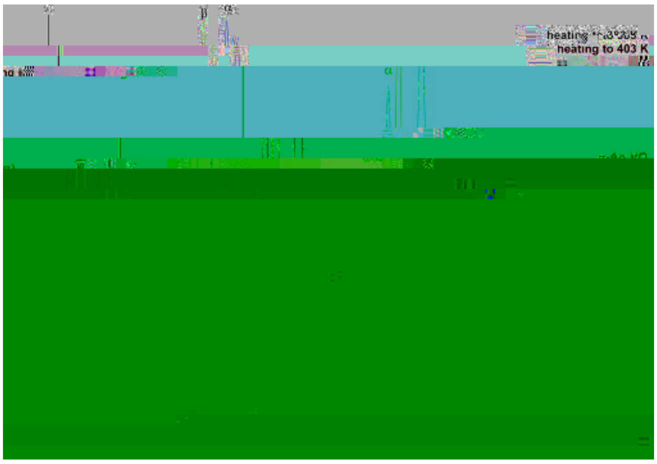
C. Crystal structures of Ag_3VO_4 and Cu_3VO_4



[illegible]

[illegible] 0 [illegible] −1.01 V [illegible]

[illegible]



[illegible]

[illegible]

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

[illegible]

[illegible] [32,33] [illegible]

[illegible]

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