

Intrinsic Defect Center in Ternary Chalcogenide Semiconductor

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I-III-VI₂ II-VI
 CuInSe₂ CuGaSe₂
 CuInSe₂
 G

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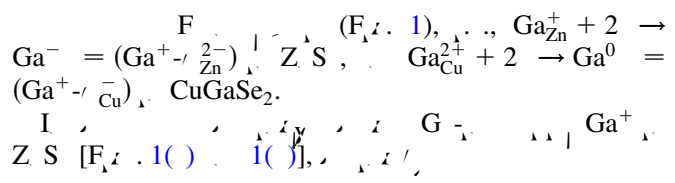
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VI

F I G
 C B Z S
 I-III-VI₂ II-VI
 Z O W F
 F A II-
 ZnO CdS Cu(In, Ga)Se₂ [5]
 In_{Cu} Ga_{Cu}
 Cu₂ [5,10], DE

CuInSe₂ CuGaSe₂
 intrinsic
 T C (I) G (III)
 CuGaSe₂ F
 I CuInSe₂-CuGaSe₂ [5]
 T I-III-VI₂
 CuInSe₂ [6-8] I -C (In_{Cu})
 CuInSe₂ CuGaSe₂
 C - Cu [6,7,9], ()
 (In_{Cu}-2/ Cu) [10]
 ()
 [11,12], ()
 [13]. W
 intrinsic In_{Cu}²⁺
 Ga_{Cu}²⁺ CuInSe₂ CuGaSe₂

R [7]. I
 LDA (VBM) LDA + [13],
 (CBM). I R [16].
 The Frenkel-pair character of the center.— T,
 II-VI Z S :G [11]
 -III GaZn [17]. T,
 F Ga_{Cu} CuGaSe₂ In_{Cu}
 CuInSe₂
 Z S CuGaSe₂. (N Z S CuGaSe₂
 C G) I



(F.1.2). *single-particle* ϵ \mathbb{F} $\mathbb{W} \parallel \mathbb{K}$

$\varepsilon = \dots$ (Fig. 2). B
 \dots PL,
 \dots
 $\text{In}^0 \rightarrow \text{In}^+ + \dots$
 $(\text{abs} = 0.81 \text{ eV}). (\dots) \text{T}$