

Intrinsic Defect Center in Ternary Chalcogenide Semiconductor

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

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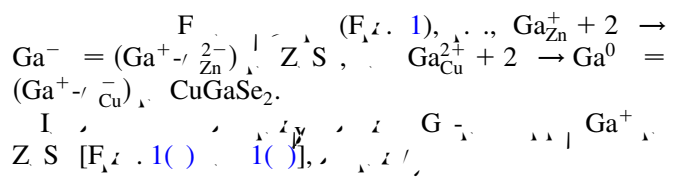
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VI

F B I G
I-III-VI₂ II-VI Z S
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
C (I) G (III)
CuGaSe₂
I CuInSe₂-CuGaSe₂ [5],
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

LDA R [7]. I
(VBM) LDA + [13],
(CBM). I
R [16].
The Frenkel-pair character of the center.— T,
II-VI Z S :G
-III Ga_{Zn} [11-13]
[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} $\mathbb{W} \parallel \mathbb{F}$

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