

Intrinsic Defect Center in Ternary Chalcogenide Semiconductor

Srinivas Latha, Zhenyuan
National Renewable Energy Laboratory, Golden, Colorado 80401, USA
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I-III-VI₂ II-VI
CuInSe₂ CuGaSe₂
CuInSe₂
G

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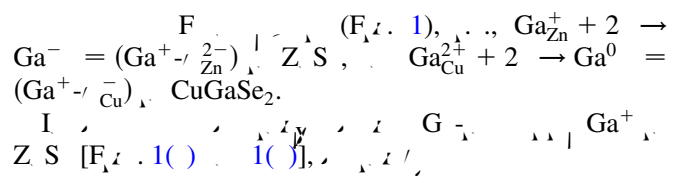
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VI

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