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 $S \rightarrow L \rightarrow H \rightarrow H \rightarrow Z \rightarrow L$ National Renewable Energy Laboratory, Golden, Colorado 80401, USA (R  $_{1}$  16 A  $_{2}$  2007;  $_{1}$  3 J  $_{2}$  2008) I III-V I II-VI **x** . A A A , 1 м y I-III-VI<sub>2</sub> CuGaSe<sub>2</sub>,  $CuInSe_2$ 1 1 \* 1 - Y 1 I N' \* \* CuInSe<sub>2</sub>-· . -1 1 1 IIV G . y DOI: 10.1103/P<sub>y</sub> R L .100.016401 PACS : 71.55.-, 61.72.B , 72.20.J , 84.60.J F y. By y G С û-√î I-III-VI<sub>2</sub> ZS м', , , , , , Z O F | | <sup>1</sup> | F | F II-. 'A` Т Ŵ ly 1, <sup>|</sup> [5], ,  $ZnO^{\circ}CdS$  Cu(In, Ga)Se<sub>2</sub> 1 . S Ш In<sub>Cu</sub> 'Ga<sub>Cu</sub> Y LIA 1 · 7. ฬ ` ` ~ [5,10],**DF** พี่ Cuy ' I · • ۱. 1 1 CuInSe<sub>2</sub>  $CuGaSe_2$ , intrinsic 11 ·y ١Y C (I) G (III) · y, CuGaSe<sub>2</sub>, 1 , F 1- 1 I  $CuInSe_2$ -CuGaSe $_2$   $\downarrow$   $\downarrow$   $\chi$ ¥ ¥ 114 у y LDA + W W П (VBM) [13], ¥. v I-III-VI<sub>2</sub> (CBM). I 1. I () I , *I* R . [16]. y I - C'(In<sub>Cu</sub>)The Frenkel-pair character of the center. — T.  $CuInSe_{2} \begin{bmatrix} 6 & 8 \end{bmatrix}$  $\begin{bmatrix} Z & S & :G \\ & & \\ & & \end{bmatrix}^{I} = \begin{bmatrix} Z & S & :G \\ & & & \\ & & & Ga_{Zn} \end{bmatrix} \xrightarrow{I} \xrightarrow{I} \xrightarrow{I} \begin{bmatrix} \overline{I} & \overline{I} \\ \overline{I} & \overline{I} \end{bmatrix}$ CuInSe<sub>2</sub> CuGaSe<sub>2</sub> , II-VI / <sub>Cu</sub> [6,7,9], (,) , I 1 1  $(In_{Cu}-2/Cu)$  [10] × vi . I [17]. T F Ga<sub>Cu</sub>, CuGaSe<sub>2</sub> · • • • • • • N In<sub>Cu</sub> 1 [11,12], ( ) , , , Y. Y CuInSe<sub>2</sub> . <sub>1</sub> <sup>7</sup> ี่ พ่ ` [13]. W , , <sup>M</sup>, \_l× , Y z, s<sup>1,2</sup>, ' CuGaSe<sub>2</sub>. (N ŢZŠ<sup>₩</sup> CuGaSe<sub>2</sub> ~ ` · | Ž CuGaSe<sub>2</sub> CuInSe<sub>2</sub> 1"  $\mathbf{C} \stackrel{\mathbf{I}}{=} \stackrel{\mathbf{V}}{\mathbf{G}} .)^{\mathbf{I}} \mathbf{I}$ - , - , · · · · · · · · , , × ¥ x ¥ .

0031-9007 08 100(1) 016401(4)

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 $F \qquad (F_{L} \cdot 1), \dots, Ga_{Zn}^{+} + 2 \rightarrow Ga^{-} = (Ga^{+} - \frac{2}{Zn}) \prod_{i=1}^{l} Z_{i} S \qquad (Ga_{Cu}^{2+} + 2 \rightarrow Ga^{0}) = (Ga^{+} - \frac{2}{Cu}) \prod_{i=1}^{l} CuGaSe_{2}.$   $I \qquad (Ga^{+} - \frac{2}{Cu}) \prod_{i=1}^{l} CuGaSe_{2}.$   $I \qquad (Ga^{+} - \frac{2}{Cu}) \prod_{i=1}^{l} CuGaSe_{i} \qquad (Ga^{+} - \frac{2}{Cu}) \prod_{i=1}^{l} Ga^{+} \prod_{i=1}^{l}$ 

 $(F_{1}, 2), C \xrightarrow{i}_{1}, i \xrightarrow{i}_{2}, i \xrightarrow{i}_{3}, i \xrightarrow{i}_{4}, i \xrightarrow{i}_{5}, F \xrightarrow{i}_{1}, i \xrightarrow{i}_{5}, i \xrightarrow{$