



**Figure 13.7** Electronic levels of intrinsic defects in CuInSe<sub>2</sub>. On the left side the theoretical values are presented and on the right side experimentally reported values are presented. The height of the histogram columns on the right side represents the spread in experimental data. (From Zhang S, Wei S, Zunger A, Katayama-Yoshida H, *Phys. Rev. B* **57**, 9642–9656 (1998) [47])

**Table 13.2** The most important intrinsic defects for device-quality CuInSe<sub>2</sub>

Defect	Energy position	Type
$V_{\text{Cu}}$	$E_{\text{V}} + 0.03 \text{ eV}$	Shallow acceptor
$\text{In}_{\text{Cu}}$	$E_{\text{C}} - 0.25 \text{ eV}$	Compensating donor
$V_{\text{Se}}$		Compensating donor
$\text{Cu}_{\text{In}}$	$E_{\text{V}} + 0.29 \text{ eV}$	Recombination center

The effect of Ga on the electronic and defect properties is discussed in Reference [36]. In those calculations, acceptor levels did not differ very much between CuInSe<sub>2</sub> and CuGaSe<sub>2</sub>, but the donor levels are deeper in the Ga-containing compound. This is consistent with observations of increased *p*-type conductivity at high Ga-concentrations [48]. At typical device compositions,  $\text{Ga}/(\text{Ga} + \text{In}) < 0.3$ , any effect of increased Ga content on conductivity has not been verified.

### 13.2.4 The Surface and Grain Boundaries

The surface morphology and grain structure are most commonly characterized by scanning electron microscopy (SEM), but transmission electron microscopy (TEM) and atomic force microscopy have also proved valuable. A typical SEM image is shown in Figure 13.8 and a TEM cross-sectional image in Figure 13.2. In general, the films used in devices