A Sum Rule for Deep Centers in II-VI Semiconductors

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Several well-known deep centers in II-VI semiconductors have more than one energy level within the forbidden gap.[1] Radiative transitions often occur in such centers between these levels as well as via charge transfer processes[2]. It has also been proposed to explain the existence of narrow zero-phonon lines in the charge transfer region in terms of bound exciton transitions[3]. We have investigated typical examples of such centers in ZnS and CdS and have observed that the energy of the zero-phonon lines of the two above mentioned transitions sum up in many cases to a value near the band edge energy. ZnS:Cu e.g. emits at 2 K a blue band with a zero phonon energy ω_1 = 2.965 eV and an infrared line ω_2 = 0.858 eV. This results in $\omega_1 + \omega_2$ = 3.823 eV which is very near the known value of the band edge energy of ΔE = 3.83 eV. Other examples of this sum rule are given in Table 1. A possible explanation of such a rule is that the charge transfer like transitions consist of the simultaneous excitation or recombination of a bound electron and hole in an excited state of the multilevel center. Then a deeply bound exciton can exist with a binding energy almost equal to the separation energy of the two inner levels of the center.

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Table 1

	ω_1 [eV]	ω_2 [eV]	$\omega_1 + \omega_2$ [eV]
CdS:Cu	1.777	0.773[4]	2.55
ZnS:Cu	2.965[5]	0.858[4]	3.823
ZnS:Ni[5]	2.4377	1.406	3.844
ZnS:M center[5]	2.3332	1.5123	3.8455