ERRATA

Erratum: Origin of the deep center photoluminescence in $CuGaSe_2$ and $CuInS_2$ crystals [J. Appl. Phys. 86, 364 (1999)]

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In Ref. 1 the photoluminescence due to electron-hole recombination via deep donor–acceptor pairs (DAP's) in $CuGaSe_2$ and in $CuInS_2$ crystals was investigated experimentally. For the emission spectrum analysis it was stated that, for otherwise similar pairs but with the donor–acceptor separation varying—r_1 and r_2, respectively—a difference ΔE_{12} in the emission energies would be expected

$$\Delta E_{12}=\frac{Z_D Z_A e^2}{\epsilon}\left(\frac{1}{r_1}-\frac{1}{r_2}\right). \tag{1}$$

Here Z_D denotes the charge number of the donor, and Z_A that of the acceptor atom, e is the electronic charge, r_1 and r_2 are the pair separations, and ϵ the dielectric permittivity. As discussed below, herein lies an error which we presently want to correct.

The Coulomb term of Eq. (1) derives from the electrostatic interaction between the donor and the acceptor ''sites.'' It is known that the electron (hole) wave function of the deep donor (acceptor) level is, as a rule, highly localized. We may thus assume that just prior to the recombination emission the donor state of the DAP-complex will have a charge number of Z_D and that the charge number of the acceptor, with spatial separation r_i from the donor, will be Z_A. Thus, the contribution of the Coulomb interaction to the total energy of the excited state of the DAP complex will be $E_C^{\mathrm{ex}}(r_i)=Z_D Z_A e^2/(1/\epsilon r_i)$. For the ground state, i.e., immediately after the recombination, an electron is transferred from the donor site to the acceptor site, so the Coulomb term now becomes $E_C^{\mathrm{gr}}(r_i)=(Z_D+1)(Z_A-1)e^2/(1/\epsilon r_i)$. It is the difference in these two electrostatic energies, $\delta E_i=E_C^{\mathrm{ex}}(r_i)-E_C^{\mathrm{gr}}(r_i)=(Z_D-Z_A+1)e^2/(1/\epsilon r_i)$, which is carried over into the energy $h\nu$ of the electromagnetic quantum emitted as a result of the *eh*-recombination. From this it follows that the spectral splittings, between two different donor–acceptor separations, r_1 and r_2, will not be given by Eq. (1) but by

$$\Delta E_{12}=\frac{(Z_D-Z_A+1)e^2}{\epsilon}\left(\frac{1}{r_1}-\frac{1}{r_2}\right). \tag{2}$$

For two nonionized DAP component atoms $Z_D=Z_A=0$, the ''charge multiplier'' is thus $(Z_D-Z_A+1)=1$. This yields the formula usually employed in data analysis:

$$\Delta E_{12}=\frac{e^2}{\epsilon}\left(\frac{1}{r_1}-\frac{1}{r_2}\right). \tag{3}$$

The correction discussed presently [i.e., Eq. (2)] does not result in any change in our previous interpretation, cf. Ref. 1, which was indeed based on Eq. (3). Nevertheless, it is worth emphasizing that in the most general case the overall charge neutrality of the DAP close pair complex, i.e., for the excited state of the recombination center, cannot always be taken for granted. Either DAP atom—or both of the atoms—might, in fact, be ionized. From the experimenter's point of view, this will have some crucial consequences:

(i) When performing the data analysis, close attention should be paid to the multiplier (Z_D-Z_A+1), with every effort taken in order to ensure that correct (integer) numbers Z_D, Z_A are chosen. This may be regarded as an added complication.

(ii)There is the upside of the coin, also. It is clear that, at least in principle, the factor (Z_D-Z_A+1) provides—when

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the experimental conditions are suitable—an added degree of freedom for the interpretation of the data. In some cases $(Z_D - Z_A + 1) = 0$. If this is, indeed, the case, no ΔE_{ij} ladder of Eq. (2)—or of Eq. (3)—should be visible in the deep emission spectrum.

(iii) Finally, the ''exotic'' possibility that the factor $(Z_D - Z_A + 1) < 0$ might not be totally excluded. In this case, on the energy scale, the direction of the ΔE_{ij} ladder is reversed: *i.e., the quantum emission energy $h\nu$ will increase for increasing pair separation*. Thus, the closest pair emission will occur at the lowest energy (and not at the highest) of the series, contrary to what has been assumed to be the rule rather generally.

Finally, we once more emphasize that the present correction does not change our conclusions of the structure of the close pair DAP complexes in $CuGaSe_2$ and $CuInS_2$, as presented in Ref. 1.

[1] J. Krustok, J. H. Schön, H. Collan, M. Yakushev, J. Mädasson, and E. Bucher, J. Appl. Phys. **86**, 364 (1999).