Erratum: Excitonic and biexcitonic properties of single GaN quantum dots modeled by 8-band k · p theory and configuration-interaction method [Phys. Rev. B 79, 245330 (2009)]

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After publication of this paper we discovered that one of the parameters, i.e., the d_{15} piezoelectric constant of wurtzite materials, was wrongly taken to be positive for both GaN and AlN materials, while it should be negative.¹ Recent *ab initio* calculations reveal conclusively that the sign of d_{15} is negative for both GaN and AlN. In the literature, both positive^{2,3} and negative^{4,5} values of d_{15} have been reported, but it was identified¹ that this is a result of a misprint contained in the paper by Muensit *et al.*² when reporting the experimental values from Tsubouchi and Mikoshiba.⁴ The frequently cited work of Bernardini and Fiorentini³ reported the value of Muensit *et al.*² rather than the original experimental work, and because many authors referred to their work³ when listing piezoelectric coefficients, the error propagated. The compilation from Vurgaftman and Meyer⁶ also contains the erroneous positive sign.

Taking into account the correct negative sign for d_{15} , i.e., $d_{15} = -0.326$ and -0.418 C/m^2 , for GaN and AlN, respectively, we have recalculated the results presented in our original Fig. 8 and the corrected results are shown here: the dependence of the biexciton shift B_{XX} on exciton energy for GaN and AlN quantum dots (QDs). The B_{XX} value is a very sensitive measure of interplay between electron confinement, the effect of internal fields, and correlations between many electrons in the system. As can be seen in Fig. 8 below, our findings suggest that even the correct sign of the linear piezoelectric coefficient d_{15} is not enough to bring $B_{XX} < 0$ (and predict the bound biexcitons that were observed experimentally⁷), unless manually reduced at least to $\sim 1/3$ of its nominal value (as we concluded in our original paper). We would like to emphasize that the inclusion of higher-order piezoelectric effects may possibly compensate for the very strong effect of linear piezoelectric coefficients in wurtzite nanostructures and yield negative B_{XX} values.



FIG. 8. (Color online) The dependence of biexciton shift on exciton energy for quantum dots with D/h = 3, $h \in (1, 1, 2, 1, 4, 1, 6, 1, 8, 2, 3, 4)$ nm, and spontaneous polarization multiplied by *a* and piezoelectric polarization multiplied by *b* in the cases: (a) a = 1, b = 1; (b) a = 1/3, b = 0; (c) a = 0, b = 1/3; (d) a = 0, b = 0 (for the notation see the text in the original paper). CI calculation with $N_e = 8$ electron and $N_h = 14$ hole states: with wrong $d_{15} > 0$ as in original paper (solid lines with dots) and with correct $d_{15} < 0$ (solid lines with triangles) in addition to $N_e = 2$, $N_h = 2$ (dashed lines) corresponding to the Hartree approximation is presented. In (c) the height of the QD for the end points is specified and is the same for all four graphs. The inset in (d) depicts topmost (eighth) electron and lowermost (14th) hole state used in CI calculations for the smallest QD in the series (D = 3 nm and h = 1 nm) that are still well localized to the QD region.

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- ¹J. Pal, G. Tse, V. Haxha, M. A. Migliorato, and S. Tomić, Phys. Rev. B **84**, 085211 (2011).
- ²S. Muensit, E. M. Goldys, and I. L. Guy, Appl. Phys. Lett. **75**, 4133 (1999).
- ³F. Bernardini and V. Fiorentini, Appl. Phys. Lett. **80**, 4145 (2002).
- ⁴K. Tsubouchi and N. Mikoshiba, IEEE Trans. Sonics Ultrason. **SU-32**, 634 (1985).
- ⁵K. Shimada, Jpn. J. Appl. Phys. **45**, L358 (2006).
- ⁶I. Vurgaftman and J. R. Meyer, J. Appl. Phys. **94**, 3675 (2003).
- ⁷D. Simeonov, A. Dussaigne, R. Butté, and N. Grandjean, Phys. Rev. B **77**, 075306 (2008).