Sauer and Thonke Reply: In a recent Letter [1] we showed by very low noise cathodoluminescence measurements and an evaluation procedure using derivatives of the measured spectra that the free exciton (FE) in diamond is split into two similar groups of lines spaced by a main splitting of $\approx$10.3 meV. This finding was novel, being incompatible with previous reports on the excitonic fine structure; an interpretation of the doublet splitting was needed. Two basic interactions suggested themselves, spin-orbit and spin-spin (exchange) interaction.

In a paper [2] preceding our Letter [1] the authors of the Comment [3] theoretically demonstrated that the spin-orbit splitting λ_0 [4] of the valence band (Γ_8^+ and Γ_7^+ hole states) calculated *ab initio* to be $\lambda_0 = 13$ meV [5] is reduced to $\lambda_{exc} \approx 8.6$ meV for the FE, and farther down to $\lambda_B \approx 3.9$ meV for the hole bound to the acceptor boron. Consequently, we noted [1] that "with improved computational accuracy it appears possible, to associate the observed FE splitting with the spin-orbit interaction λ_{exc}"—as suggested in the Comment.

However, given the strong reduction of the spin-orbit interaction energy λ with increasing binding of the hole [2] a discrepancy arises with the fine structure of the boron bound exciton (BE). Here the exciton, with an electron-hole binding energy of $\approx$80 meV, experiences an additional localization energy to the neutral acceptor of $\approx$55 meV [6] which is mediated by the two holes close to the acceptor ion. The BE recombination spectrum also reveals a splitting into two groups of lines, with a main doublet spacing of $\approx$11 meV [7]. This spectral structure is surprisingly similar to that of the FE [8]. Assuming explicitly that the similar fine structures of the FE and BE spectra have the same generic origin [1] we found it unreasonable to ascribe the doublet splittings, in both cases close to 11 meV, to the spin-orbit interaction. Interestingly, this was also stated distinctly by Serrano *et al.* [2] based on their calculations: "We found no obvious way of relating to spin-orbit coupling the splitting of 12 meV observed for the exciton bound to neutral acceptors."

This situation motivated us to search for different explanations of the $\approx$11 meV fine structure splitting. It was shown by intuitive physical arguments and comparison to the helium atom that the experimental data are *consistent* with a model of spin singlet and triplet excitons.

To summarize, the interpretation of the exciton doublet splitting is by no means clear contrary to the statement in the Comment: Either the experimental similarity of the fine structures of the FE and BE spectra is completely accidental (in this case the arguments of the Comment may apply and seem to establish a rather persuasive picture for the FE, with no implication for the BE) or the similarity represents an equivalent physical situation for both complexes. In this case, the interpretation advanced in the Comment would not apply, or the trends calculated by Serrano *et al.* [2] on which we have relied are not realistic even on a very gross scale.

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Received 28 November 2000
DOI: 10.1103/PhysRevLett.86.3924
PACS numbers: 71.35.–y, 71.55.Ht, 78.60.Hk

[1] R. Sauer, H. Sternschulte, S. Wahl, K. Thonke, and T. R. Anthony, Phys. Rev. Lett. **84**, 4172 (2000).
[2] J. Serrano, M. Cardona, and T. Ruf, Solid State Commun. **113**, 411 (2000).
[3] M. Cardona, T. Ruf, and J. Serrano, preceding Comment, Phys. Rev. Lett. **86**, 3923 (2001).
[4] Confusion may emerge from the different notations in Refs. [1,2] and the Comment: In Refs. [1,2], the spin-orbit interaction energy was labeled Δ with an additional index to distinguish between free holes and holes bound in free or localized excitons. In the Comment, the spin-orbit interaction energy is denoted by λ, and Δ is the exchange interaction energy. Throughout this Reply we will refer to the latter notation.
[5] M. Willatzen, M. Cardona, and N. E. Christensen, Phys. Rev B **50**, 18 054 (1994).
[6] P. J. Dean, E. C. Lightowlers, and D. R. Wight, Phys. Rev. **140**, A352 (1965).
[7] H. Sternschulte, S. Wahl, K. Thonke, R. Sauer, T. Ruf, M. Cardona, and T. R. Anthony, Mater. Sci. Forum **258**, 1113 (1997).
[8] To show this important fact with details of the splitting clearly we reproduced Fig. 2 from the original Ref. [7] as cited in [1].

 0031-9007/01/86(17)/3924(1)$15.00