Reply to "Comment on 'Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theory'"

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We thank Prof. Sevilla for his comments on our paper. We agree with the comments. The LC-functionals, including CAM-B3LYP, do indeed predict the HOMO of the AT base pair to be located on adenine. We erroneously assigned the orbital involved in the lowest transition calculated using the LC-functionals to the HOMO. The orbital involved is in fact the HOMO−1 and that is the orbital plotted in Figure 1 and in TOC figure. The text describing Figure 1 should read: *This is illustrated in Figure 1 where we plot the HOMO and LUMO of the AT base pair as obtained using B3LYP and the HOMO−1 and LUMO calculated using CAM-B3LYP. We see that B3LYP predicts that the lowest transition occurs from the HOMO located on adenine to the LUMO on thymine, whereas CAM-B3LYP (and the other LC functionals) correctly predicts that the transitions are from the HOMO−1 to the LUMO both located on the thymine unit. Thus, the wrong result predicted by B3LYP is due to an underestimation of the highest occupied adenine orbital relative to thymine in the base pair.* Likewise, in Figure 1 and the TOC figure, the orbital for the LC-functional should be HOMO−1 not the HOMO orbital. The conclusions of the paper remain the same.

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