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Charge Transfer States of Aqueous B-DNA at Energies Above the Bright $^1\pi\pi^*$ Exciton States ADRIAN LANGE, Chemistry Dept. (Physical), JOHN HERBERT, Chemistry Dept. — Charge transfer states have been proposed to explain experimentally observed long-lived excited state dynamics in aqueous DNA oligomers[1]. Due to the large number of atoms, tractably describing such excited states in DNA systems with *ab initio* theory is limited to TD-DFT. However, standard TD-DFT exchange-correlation functionals significantly underestimate CT excitation energies owing to incorrect asymptotic behavior. To circumvent this error, we instead apply recently developed and optimized long-range corrected TD-DFT functionals to better assess the low lying CT and exciton states of DNA oligomers. We show that long-range corrected TD-DFT yields results comparable to correlated wave function models, placing CT states of aqueous B-DNA at energies above the optically bright $^1\pi\pi^*$ exciton states, contrary to TD-DFT results which find CT states below the exciton states.

[1]Crespo-Hernández, C. E.; Cohen, B.;Kohler, B. *Nature* **2005**, *436*, 1141.

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