DETERMINATION OF EXCITON LENGTH IN AQUEOUS B-DNA USING LONG-RANGE-CORRECTED TIME-DEPENDENT DENSITY FUNCTIONAL THEORY(LRC-TDDFT)

RYAN M. RICHARD, JOHN M. HERBERT, *Department of Chemistry, The Ohio State University, Columbus, OH 43210.*

In our present work, we are interested in the excited state dynamics of four explicit solutes, all of which are polyadenine B-DNA derivatives, which range in size from two to four adenine bases. Of all the excited state properties these systems possess, we have specific interest in determining the exciton length as this has been an area of debate in the literature. In order to accurately calculate the exciton length, we explore the use of both implicit and explicit solvation on the system by means of a polarizable continuum model (PCM) and a combined quantum mechanical/molecular mechanical model (QM/MM). For both solvation models the solute particles are treated with LRC-TDDFT, specifically we make use of two "long-range corrected" (LRC) density functionals developed previously in our group, LRC-ωPBE and LRC-ωPBEh. Previous comparisons to *ab initio* benchmarks have shown that these functionals provide a consistent treatment of both localized and charge-transfer excited states within TDDFT.