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Calculation of the optical response of biomolecules using TDDFT
ARGYRIOS TSOLAKIDIS, EFTHIMIOS KAXIRAS, Department of Physics, Harvard University — We present calculations of the optical response of various biomolecules, using time-dependent density functional theory (TDDFT). These calculations are performed in real time within the adiabatic approximation with a basis of local orbitals. First we study the DNA bases and base-pairs both in their normal and tautomeric forms in the gas phase. Our results for the individual bases are in good agreement with experiment and computationally more demanding calculations of chemical accuracy. The optical response of base pairs indicates that the differences between normal and tautomeric forms in certain cases are significant enough to provide a means of identification. The second part of our work deals with the effect of hydration on the absorption spectrum of the aromatic amino acids Tryptophan, Phenylalanine and Tyrosine. We discuss the changes that occur with the inclusion of several water molecules and compare with experiment and other theoretical calculations.

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