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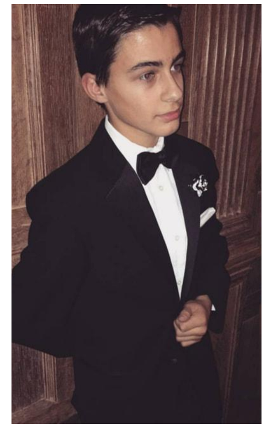
Title: An Investigation of the Vibrational and Electronic Effects on the Efficiency of Electron Transfer in Photosynthesis Using a Density Functional Theory Simulation



Abstract

Photosynthesis is the process by which many autotrophic organisms, notably plants, convert energy from electromagnetic radiation into a more useful, chemical form. This process, occurring largely due to the pigment chlorophyll, is very efficient despite the chaotic environment in most biological systems where electrons may lose energy or be lost when causing damage through interactions with the proteins. The efficiency in photosynthesis originates from quantum mechanical phenomena, as proven by experimental data, so the effect with the greatest impact on efficiency would also have the greatest impact on maintaining coherence in chaotic environments. I performed Density functional theory simulations of Chlorophyll-a and Chlorophyll-b at various temperatures and in various environments to distinguish which effect, vibrational or electronic, has the greatest impact on photosynthetic efficiency. This included varying temperature throughout an extreme interval in which plants may live, as well as by altering the structure of the chlorophyll molecule and which solvent the chlorophyll was in. The simulations were performed using auxiliary density functional theory through the deMon-2k software on the Compute Canada computers and were compared with experimental data. The data qualitatively support that these effects impact coherence and this understanding of phenomena could be used in human-developed quantum technologies to allow coherence at higher temperatures and more chaotic environments including photovoltaic cells and the quantum computer.