A new theoretical approach to calculating the probability of charge transfer between atomic orbitals DALE IGRAM, ERIC HEDIN, YONG JOE, Ball State University — In the world of physics, the probability of charge transfer is more commonly known as tunneling or transmission coefficient where physical parameters such as barrier height and width, and energy of incident particle are considered. However, an alternative approach based on the overlap of the wave functions of atomic orbitals has been developed. The overlap of wave functions is described by an overlap integral parameter S as a function of $pp\sigma$ and $pp\pi$ interactions. We will reveal that the probability of charge transfer is proportional to the ratio of the overlap integral S and $S_{\max}$ for two atomic orbitals. Results for several atomic orbital combinations of guanine and cytosine molecules for a B-DNA molecule are presented and discussed.

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