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**Proton transfer along water bridges in biological systems with density-functional tight-binding**[1] KRYSTLE REISS, ABIGAIL WISE, JAMES MAZZUCA, Alma College — When examining the dynamics of charge transfer in high dimensional enzymatic systems, the cost of quantum mechanical treatment of electrons increases exponentially with the size of the system. As a semi-empirical method, density-functional tight-binding aids in shortening these calculation times, but can be inaccurate in the regime where bonds are being formed and broken. To address these inaccuracies with respect to proton transfer in an enzymatic system, DFTB is being used to calculate small model systems containing only a single amino acid residue donor, represented by an imidazole molecule, and a water acceptor. When DFTB calculations are compared to B3LYP geometry calculations of the donor molecule, we observe a bond angle error on the order of 1.2 degrees and a bond length error on the order of 0.011 Å. As we move forward with small donor-acceptor systems, comparisons between DFTB and B3LYP energy profiles will provide a better clue as to what extent improvements need to be made. To improve the accuracy of the DFTB calculations, the internuclear repulsion term may be altered. This would result in energy profiles that closely resemble those produced by higher-level theory.

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