Tipping the Scales: The Affect of an Electric Bias on Proton Conduction Pathways with Kinetic Monte Carlo

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Yttrium doped $BaZrO_3$ is a promising proton conductor in fuel cells. Kinetic Monte Carlo (kMC) simulations were used to sample the infrequent events of a proton overcoming a transition state energy barrier as it moves from binding site to binding site in $Y/BaZrO_3$. However, a large percentage of the proton conduction pathways found using the standard kMC program traversed only a small portion of the simulation box before looping back on themselves. Yet, it is the fully traversing pathways that are of interest when studying conduction through the proton conducting membrane in an actual fuel cell. This study probes the effects of adding an electric bias to the system by dividing it into discrete, infinite sheets of charge and applying a potential difference between the anode and the cathode. This introduces an electrical work term into the calculation of the rate constant and effectively lowers the energy barriers for moves in the direction of the bias. By updating the program with arrays incorporating sheet charges and their resulting potentials, the simulation was modified to incorporate the new field. With the modified program, pathways with and without the bias and with different applied potential were compared. The resulting outputs were compared in terms of average time to complete a full trajectory and the number of steps taken. A potential difference of 0.012 eV/Å decreases average time per trajectory substantially.