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Electron Transfer rate calculation for electrodes with immobilized enzymes on Carbon Nanotubes ASHVIN KUMAR VASUDEVAN, GORDON.A THOMAS, REGINALD.C FARROW, ALOKIK.P KANWAL, SHACHI YADAV, New Jersey Inst of Tech — Fuel Cells are rapidly emerging as an alternate fuel source to produce power at a high efficiency. Enzymatic fuel cells provide a way to use cheap fuels while eliminating the use of metals. While the cost of the fuel cell is usually cheap, problems arise due to inefficient electron transfer from the enzyme to electrode. Our group addresses this by incorporating vertically aligned carbon nanotubes (enzymes immobilized onto them) to help promote the electron transfer. This talk deals with the theoretical calculations involved in the process. To obtain an accurate prediction of the electron transfer, the environment, the orientation of the enzyme on the electrode, distances involved in the electron transfer, type of reaction and the energies of the enzymes involved before and after the electron transfer are to be considered. The calculation follows Marcus' theory with the enzymes used, Glucose oxidase and laccase, taken as donor and acceptor. Hence to solve the electron transfer equation, the free energies, reorganization energies – inner shell and the outer shell must be found. These energies were obtained with the help of the x-ray structures found in the protein database. The parameters involved in each calculation will be reviewed.

Ashvin Kumar Vasudevan
New Jersey Inst of Tech

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