Electron transport through the building blocks of proteins

DAVID CARDAMONE, GEORGE KIRCZENOW, Department of Physics, Simon Fraser University — We investigate two-terminal charge transport through single oligopeptide molecules, thiol-bonded to gold leads. Applying ab initio and semi-empirical techniques, we calculate equilibrium and non-equilibrium results in the Landauer formalism. The conductance and current thus obtained are consistent with the recent experimental results of X. Y. Xiao, B. Q. Xu, and N. J. Tao (J. Am. Chem. Soc. 126, 5370; Angew. Chem. Int. Ed. 43, 6148). This theory furthermore provides a straightforward explanation of the striking current rectification seen in those experiments.

1This work was supported by NSERC and CIAR.