

Abstract Submitted
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Electron transport through the building blocks of proteins¹

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.

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