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Transmission and Density of States Analysis in Electron Transport for Opioid Derivatives

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Abstract

The advances in electronics aim to develop electron devices each time smaller. Among a large range of ways to develop this concept is the organic electronics and in this last area of knowledge is the molecular electronics, where single-molecules are studied as possible electronic devices [1,2]. In this work, single-molecules based on diamorphine, 3-monoacetylmorphine, 6-monoacetylmorphine and morphine were connected between Au(111) electrodes and bias voltages were applied to understand the behavior of these molecular systems as electron devices. Different molecular structures provide slightly different applied bias responses. These changes are due to the molecular geometry that provide different available molecular energy levels to the transport. To understand how these energy levels provide electrical current, the transmission through these molecules and their density of states were analyzed and these results were compared with their respective current-voltage curves in each molecular system. The results show that differences due to acetyl group in each molecule change the energy levels excited by applied bias and how these levels are available to occupancy during the electron transport through these molecules. These results shows that diamorphine (heroin) and 3-monocetylmorphine have possible application as molecular diodes and Field Effect Transistors [3].

Key-words: Electron Transport; Transmission; Density of States; Opioid Derivatives.

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