

# WREN – WORKSHOP ON RENEWABLE ENERGIES AND NANOTECHNOLOGY - 2019

## Electronic Transport Properties of Phospholipids Molecular Devices

SIQUEIRA, M. R. S.<sup>1</sup>, OLIVEIRA, W. D.<sup>2</sup>, GESTER R. M.<sup>3</sup>, BELO, E. A.<sup>4</sup>; FERREIRA D. F. S.<sup>5</sup>; NETO A. M. J. C.<sup>6</sup>; DEL NERO J.<sup>6</sup>

<sup>1</sup> *Coordenação do Curso de Física, Universidade Federal do Amapá, Macapá, AP, Brasil.*

<sup>2</sup> *Coordenação do Curso de Engenharia Elétrica, Universidade Federal do Amapá, Macapá, AP, Brasil.*

<sup>3</sup> *Faculdade de Física, Universidade Federal do Sul e Sudeste do Pará, Marabá, PA, Brasil.*

<sup>4</sup> *Faculdade de Engenharia Mecânica, Universidade Federal do Pará, Tucuruí, PA, Brasil.*

<sup>5</sup> *Programa de Pós-Graduação em Engenharia Elétrica, Universidade Federal do Pará, Tucuruí, PA, Brasil.*

<sup>6</sup> *Faculdade de Física, Universidade Federal do Pará, Belém, PA, Brasil.*

### Abstract

Phospholipids are important components of cell membranes and have molecular structure with different centers of positive and negative charges.. They have two large tails of hydrophobic fatty acids and a hydrophilic (polar) head containing phosphate. This kind of structure indicates applications in molecular electronics as molecular diodes, Molecular Field Effect Transistors and Oscillators, providing economy of energy due to their small dimensions and quantum electronics effects. In this present work, we have studied theoretically the electronic properties of cholesterol, cortisol and testosterone attached in Au(111) electrodes using the NEGF-DFT formalism as implemented in the (Tran)SIESTA package. As expected, our results show that a simple change in geometry or composition significantly alters the molecular behavior in response to the extraneous field. While cholesterol is an isolator, cortisol and testosterone have potential applications as resonant oscillator and diode, respectively. These results are consistent with previous work and will help to understand both the applications in molecular electronics and its interactions with living systems.

**Key-words:** Electronic Transport; Phospholipids; Resonant Oscillator; Molecular Diode.