SiPrEMo – A SIMULATOR OF THE ELECTRONIC PROPERTIES OF MOLECULES

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ABSTRACT

SiPrEMo (*Simulador de Propriedades Elétricas de Moléculas - Simulator of the Electronic Properties of Molecules*) is a software package with a user-friendly interface that simulates many important electronic properties of molecules, such as the electrostatic potential, energy levels, transmission and electric current.

The simulation of the electrostatic potential uses whether the Coulomb Law if one considers a distribution of point charges, or the Poisson equation if one considers a continuum distribution of charges. The work area is fragmented in a matrix of changeable order and the potential is calculated on each cell of the matrix.

The plots of Transmission × Energy and Electric Current × Voltage are generated using Green's Functions via the Dyson Equation. The Hamiltonian matrix is generated using the extended Hückel method.

1. INTRODUCTION

The trend for shrinking the size of electronic components has been pushing researchers into the nanotechnology arena.

In this area of research, computer simulation plays a major role in finding molecules whose physical properties meet the requirements of some specific application.

In the search for these molecular devices, it is appropriate to use computational simulation where the numerical computation comes into play to help us to obtain information that one would hardly obtain in any other way.

2. THE SIMULATOR

The simulator was developed in an integrated development environment (IDE) and rapid applications development (RAD). The development of the simulator was extremely laborious even with the easiness offered by these platforms. This happens because these applications help only specifically the visual aspects of programming. The mathematical formulations of the methods are the same. The programming language used to develop the simulator was C++.

The available atoms for using in the simulator are: Hydrogen, Oxygen, Nitrogen, Carbon, Sulfur, Silicon, Iron, Aluminum, Gold, Copper, Titanium and Zirconium.

In *Fig.1*, we can see the desktop of the simulator showing a molecule of gallic acid.

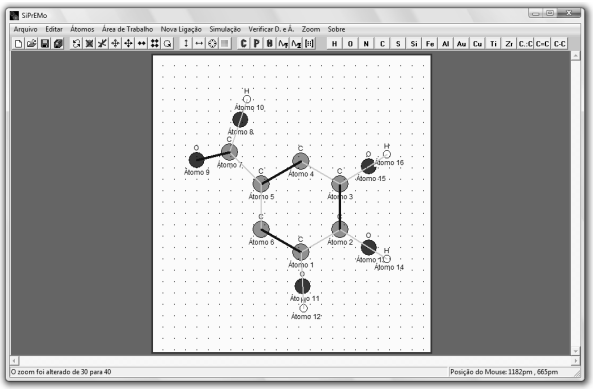

Fig. 1: Desktop of the simulator showing a molecule of gallic acid.

2.1 Coulomb Potential

One of the available simulations in SiPrEMo is the electrostatic potential calculated by a distribution of point charges according to the formula:

$$\phi_{\mathbf{E}} = \frac{q}{4\pi\epsilon_0 r} \qquad \textbf{Eq. 1}$$

The atoms are placed in a variable order matrix as point charges and the remaining cells of the matrix are filled with zeros. The calculation of the potential generated by each atom in each cell of the matrix is then initiated.

Figure 2 shows the Coulomb potential of a molecule of gallic acid.

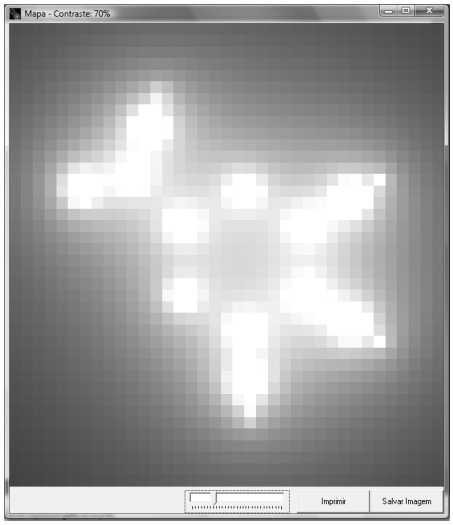

Fig. 2: Coulomb potential of a molecule of gallic acid .

After the simulation, it is possible to adjust the contrast of the output image. This facilitates the visualization of the potential distribution. It is possible to save the image in either .jpg or .bmp format. The software also calculates the error between the real distance and the numerical distance between the atoms.

2.2 The Poisson Distribution of Molecules

The simulator can determine the electrostatic potential given by the Poisson equation. At this point, the atoms are discretely distributed on a variable order matrix. In this way, however, the atoms are entered as charge densities.

Figure 3 shows the electrostatic distribution of a molecule of gallic acid using the Poisson equation.

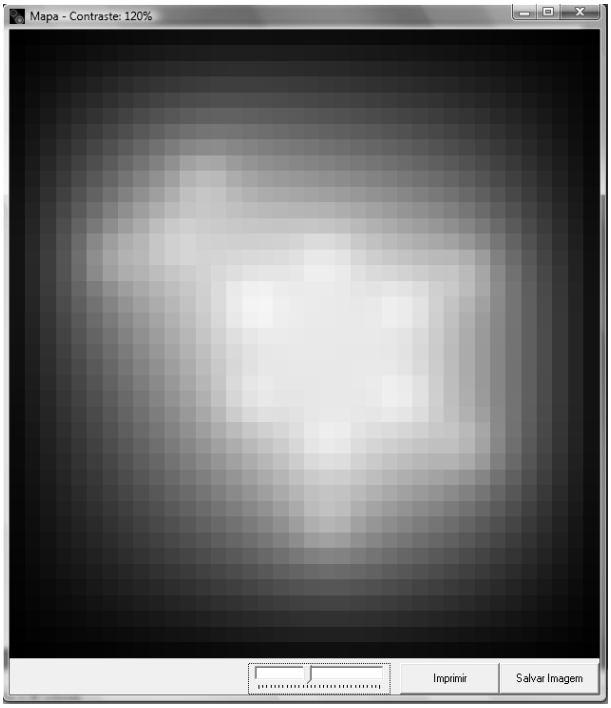

Fig. 3: Electrostatic distribution of a molecule of gallic acid using the Poisson equation.

In SiPrEMO, the successive over relaxation method is used to calculate the Poisson equation with $\lambda = 0.3\%$ and maximum tolerated error £ = 10^{-3}.

2.3 The Hückel Hamiltonian

The Hückel approximation is a simplified version of LCAO (Linear Combination of Atomic Orbitals) to find an approximated Hamiltonian for molecules.

In this method one considers only p-orbitals that are capable of forming π bonds. Other bonds are not considered because of their relative lower binding energies.

Although it is a very simplified model, the Hückel method can still be used to obtain qualitative information about energy levels of molecules.

For the Hamiltonian of a molecule of gallic acid, for instance, the matrix generated by the simulator was:

$$\begin{pmatrix}
0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.8 & 0.0 & 0.0 \\
1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.8 & 0.0 \\
0.0 & 1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.8 \\
0.0 & 0.0 & 1.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
1.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 1.0 & 0.0 & 0.0 & 0.8 & 0.8 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.8 & 2.0 & 0.0 & 0.0 & 0.0 & 0.0 \\
0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.8 & 0.0 & 2.0 & 0.0 & 0.0 & 0.0 \\
0.8 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 & 0.0 \\
0.0 & 0.8 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0 & 0.0 \\
0.0 & 0.0 & 0.8 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 2.0
\end{pmatrix} \quad \textbf{Eq. 2}$$

SiPrEMo is capable of calculating energy levels and displaying a graphic representation of them. Calculations involve the computation of eigenvalues and their associated eigenvectors.

2.4 Green's Functions

Green's functions are used to solve the Schrödinger equation numerically and to find the transmission of the system under study.

Using Green's functions, the simulator generates the Transmission × Energy plot. The software calculates a Transmission × Energy plot for a set of specific biases and then integrates them in order to find the electric current through the molecule. In this way it is also possible to obtain an Electric Current × Voltage plot.

Figure 4 shows the IV characteristic of a molecule of gallic acid.

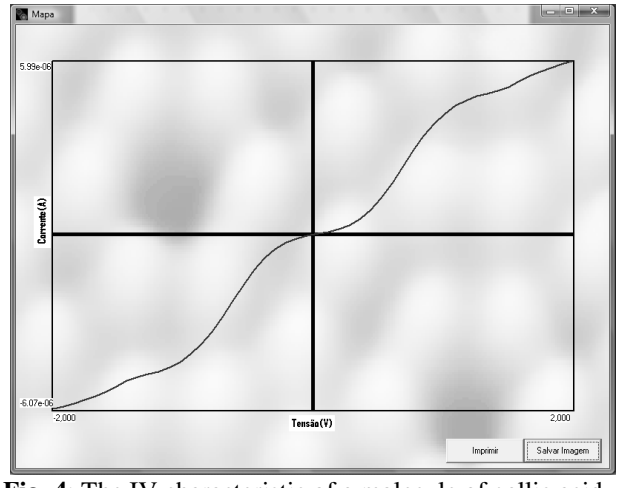

Fig. 4: The IV characteristic of a molecule of gallic acid.

3. CONCLUSIONS

A software package was developed to simulate and obtain many electronic parameters of simple molecules. The package is able to find the electrostatic distribution of molecules by means of two different techniques. Moreover, it also calculates the energy levels of

molecules by the Hückel Hamiltonian and finds the IV characteristic of a molecule based on Green's functions.

4. REFERENCES

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