

## Comparative study of the photochemical properties of silole, thiophene and furan

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The development of new organics semiconductors materials has attracted a large interest due to its application in OLEDs, LCDs and photovoltaic cells. The use of these materials enables the manufacturing of thinner and more flexible displays, portable solar cells and have been used extensively in the manufacture of electronic products [1-3]. Studies indicate that silole-containing polymers could present increased efficiency [4,5]. Despite this, the photochemistry of the silole unit and its specific role in the photophysical mechanisms these materials undergo have not been thoroughly investigated.

In this work, a comparative study of the Potential Energy Surfaces (PESs) of silole, thiophene and furan along the ring puckering and ring opening coordinates are presented, which are usually involved in the deactivation mechanisms for five-membered rings. The surfaces were constructed with the Equation-of-Motion Coupled Cluster including simple and double excitations (EOM-CCSD) implemented in the MOLPRO package [6].

The optimized geometry, vertical excitation energies, and oscillator strength were determined with the 6-31G(d,p), cc-pVTZ and aug-cc-pVTZ basis sets. The calculated geometries are similar for the three basis sets and the first two states present wave functions of the same symmetry, oscillator forces and similar vertical excitations. For more excited states, the aug-cc-pVTZ base presents a significantly better description.

The PESs for the first ten states of silole along the ring puckering mechanism were constructed with the cc-pVTZ and aug-cc-pVTZ basis sets. The 6-31++G \*\* basis was used for the ring opening mechanism PES. In both mechanisms, we identified possible crossings between the surfaces involving the bright states, but no crossing involving the ground state were found, in contrast with those obtained for furan and thiophene.

In these preliminary studies it is not possible to relate the higher efficiency observed in polymers containing silole units *versus* those containing thiophene or furan, since the complete structure of the polymers constructed with these molecules is determinant to its properties and function. However, the results suggest that the silole



# XIX SBQT

## Simpósio Brasileiro de Química Teórica 2017

12 a 17/Nov, 2017, Águas de Lindóia/SP, Brasil

has a higher photostability compared to thiophene and furan, which is an advantage for its application in photovoltaic cells, OLEDs and similar materials.

**Key-words:** silole, photochemical and potential energy surface.

**Support:** This work has been supported by Professor Marco Antonio Chaer Nascimento (UFRJ) and Itamar Borges Junior (IME).

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