Computational Simulation of C60 Embedded in Amino Acid Ionic Liquids

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INTRODUCTION

Nowadays, ionic liquids has been employed in the most wide applications in technological fields such as chemical industry, electrochemistry, optics, environmental chemistry, medicine and nanotechnology[1]. These systems has been comprised by complexes ions maintained in an equilibrium between the electrostatic and sterical forces. However, amino acid ionic liquids (AAIL) has been attained a special attention in the scientifical community by its possibility to be added to that landscape such as one more challenge in the developments in biosensors and biomaterials[2]. In the other corner of this challenge, light fullerenes has been appointed such as a probably alternative to the development into biomedical fields, in particular, C60. But, its hydrophobicity is one of the great problems that have to be overcoming[3]. In this sense, this work explore a variety of computational methods to evaluate what is the most important chemical interactions between these two systems pledging to describe the limits of that forces.

METHODS

Semiempirical molecular dynamics method has been employing in ten AAIL that has been chosen to make interactions with the same number of HSO4- anions with and without C60 using CP2K program[4]. The NVT ensemble was chosen to produce 10ps molecular dynamics with a timestep of 1 fs in the room temperature. The geometries has been optimized by each 10 fs.

RESULTS AND DISCUSSION

We found until 15 kcal/mol of difference in the energies formation of the pairs [AAIL+][HSO4-], but until 75 kcal/mol in the conformational analysis energies variations, when we compare some conformers. During the molecular dynamics the snapshots has been showing the migration of groups to the C60 surface suggesting some chemical reactivity due a polarization of this kind of fullerene in the ionic liquids. During the simulation a huge H-bond network has been formed.

CONCLUSIONS

A complex H-bond network seem to be one the main factor of the structural stability. These structure is affected by the volume and number of these pairs the presence of C60. The C60 presented some polarization in the AAIL chemical environment turning it into a reactive specie in this medium following the trends pointed in the classical molecular dynamics of similar systems.[3]

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