Adsorption of ascorbic acid as a possible way to prevent against the oxidative damage of $\text{C}_{60}$ fullerene

U L Fulco, E L Albuquerque and M S Vasconcelos

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Following the buckminsterfullerene $\text{C}_{60}$ discovery, it was soon acknowledged that its poor solubility in polar solvents is detrimental for biological applications. To circumvent this difficulty, several routes to attach chemical groups to $\text{C}_{60}$ have been proposed leading to a wide variety of derivatives with distinct physical and chemical properties. As the cytotoxicity is a sensitive function of surface derivatization, the existence of a wide range of biologically compatible solvents improves the versatility of functionalization, thereby minimizing cytotoxicity effects. In this aspect, ascorbic acid (AsA) is timely; with the chemical formula $\text{C}_{6}\text{H}_{8}\text{O}_{6}$, whose L-enantiomer is popularly known as vitamin C, it is an organic acid with antioxidant properties. The purpose of this work is to give a complete description of AsA interaction with $\text{C}_{60}$ including the effect of its different spatial orientations relative to the $\text{C}_{60}$ molecule, as a possible way to prevent against the oxidative damage and toxicity of the latter. With the help of classical molecular dynamics, the best molecular geometry corresponding to the strongest binding of AsA adsorbed on $\text{C}_{60}$ was found. Quantum ab-initio density functional theory simulations, in both the local density and generalized gradient approximations, were carried out to estimate the AsA-$\text{C}_{60}$ binding energy. Afterward, the electron transfer between the AsA and $\text{C}_{60}$ molecules was calculated to assess the noncovalent nature of their interaction. The results of this work may stimulate further research in this direction, such as the development of chemical procedures for AsA-$\text{C}_{60}$ noncovalent functionalization and the assessment of its oxidative damage and toxicity.

Biography

U L. Fulco is a member of the Department of Biophysics, Universidade Federal do Rio Grande do Norte, in Natal-RN, Brazil. The focus of his research work is in the field of NanoBiotechnology, mainly those related with the investigation of bio-drugs delivery.

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