SELF-HEALING BEHAVIOUR ORIGINATED BY DYNAMIC COVALENT BONDS IN DIARYLBIBENZOFURANONE: A DENSITY FUNCTIONAL STUDY

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ABSTRACT

The ability to conduct a responsive behaviour of the material regarding external stimulations or environment conditions may lead to prevention and even management of damages that occurred on some applications, as an example surface coating. This is provided on polymeric materials by dynamic bonds, a class of bonds that under equilibrium conditions can break and reform selectively. This dynamic behaviour is achieved by supramolecular interactions (e.g. hydrogen bonding and π- π stacking) and also dynamic covalent bonds.
Both of these types are being studied by different research groups, with a wide range of approaches. Nonetheless, Imato et al. could achieve a unique set of conditions. Using the dimer of arylbenzofuranone (ABF), the diarylbibenzofuranone (DABBF), as cross-linker, the polymer gel synthesized was able to undergo self-healing on mild conditions at room temperature. This cross-linker, in special, was already studied due to the anomalous behaviour and antioxidant character.
In this work, *ab initio* methods were used based on the density functional theory (DFT), aiming a better comprehension of the structural and electronic properties of ABF and DABBF. As a result, the HOMO-LUMO energy difference of the former was 3.74 eV. No studies in the literature were found regarding empirical values. Nonetheless, benzofuran, with a similar structure, has a HOMO-LUMO energy difference of 4.0 eV. Using the dimer of ABF, DABBF, the HOMO-LUMO transition achieved was 3.23 eV. The empirical bond dissociation energy is 1.02 eV, while the calculated was 0.71 eV. Regarding the length of the bond responsible for the dynamic behaviour, values of 1.59 A and 1.62 A were obtained, for empirical and computational measures, respectively.