



Metal enhanced interactions of graphene with monosaccharides



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ABSTRACT

The present theoretical study proposes the enhanced interaction of nanostructures with monosaccharides. It has been demonstrated that the interactions with and without metal adsorption do in fact show that the adsorption energies change accordingly. It is important to note that the chemistry of reactions can also be influenced as a result of this change in dynamics.

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1. Introduction

Graphene has been referenced a lot in recent literature whereby numerous theoretical studies [1,2]. It has been demonstrated that in the Li⁺ case, a charge of $\sim 0.8e$ is transferred to the surface of the fullerene (C₆₀) molecule [3] and small graphene sheets [1]. Modification of the surface electron configuration was also shown to yield increased reactivity. There has been many similar studies on nanotubes [4–6] by the adsorption of metal ions can influence chemistry of the graphene based system.

We shall find as central result of this letter that metal adsorption has an effect on the ability of sugars to adsorb to the surface. This effect can be explained in terms of a qualitative discussion of bond stretching while results on quasi 1-D molecules such as polyacenes and polyphenyls showing similar distortions may indicate some quantum-phase transition, which is hidden by the fact that adsorption happens in finite steps.

In previous studies [7] the interaction between various carbohydrates and a fragment of zigzag (10,0) CNT has been shown to be favourable and exothermic in the range of -6 to -8 kcal/mol. What is important to gain from our analysis is that the interaction energies do change upon adsorption of the metal ions that helps to reinforce the concept that this adsorption will play a key role for surface chemistry.

2. Computational methods

The quantum chemical calculations performed in this work on all structures were done by closing the sheets with hydrogen

atoms as we assume finite conditions. The GAUSSIAN 03 [8] codes were used. Since the systems are relatively large the geometry optimizations were performed with the Density functional theory (DFT) B3LYP method. The basis set used is the 6-31+G* for optimizations and single point energy evaluations. All calculations were verified to ensure stability of the systems obtained.

3. Results and discussion

All optimized structures for the calculations are presented (Figures 1–3) whereby selected geometrical parameters shown for optimized structures without Li (A) and with Li (B) whereby angles are shown in angles (°) and bond distances in angstroms (Å). The structures are denoted as glucose (1), fructose (2), galactose (3), mannose (4) and ribose (5). And in the table (Table 1) relative dissociation energies in kcal/mol where a. is without metal adsorption and b. is with metal adsorption. The energies shown are at the B3LYP/6-31+G* level of theory with optimizations of the stable structures.

From the dissociation energies we can observe that for glucose without the metal we obtain a value of 4.10 kcal/mol which if we look at the result of the system with Li it is higher at 4.66 kcal/mol and actually endothermic. This means that it actually requires less energy to dissociate relative to that without the metal. The electronic transfer properties of the Li are maintained which is encouraging.

For next system, fructose, the dissociation energy without the metal is -4.07 kcal/mol that is within error of the calculations themselves. This essentially means that the systems would in fact repel each other. After exposure to the metal we can see an increase to 4.45 kcal/mol which is similar to that seen for glucose which is logical given the similarity in molecular structure.

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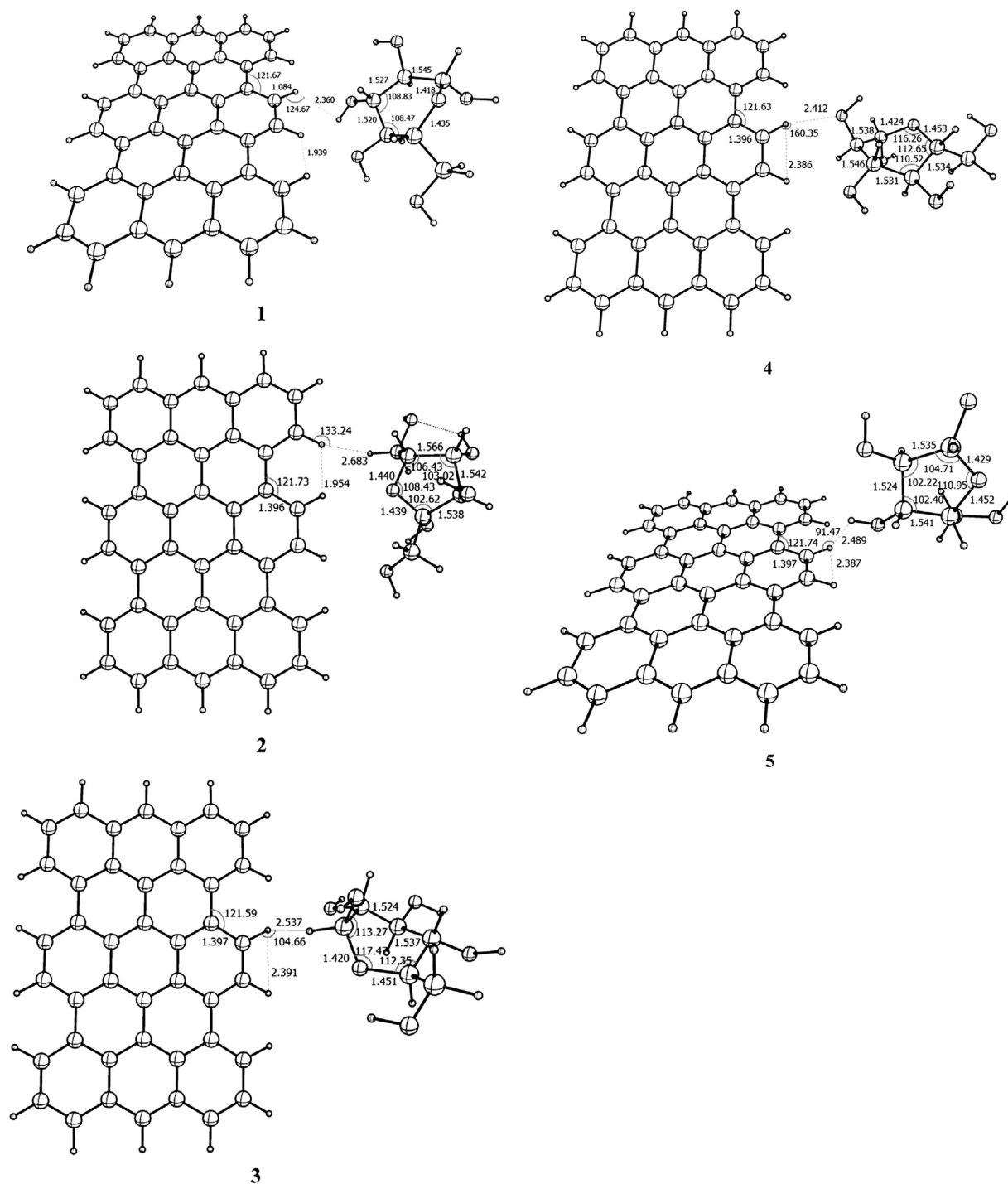


Figure 1. Selected geometrical parameters optimized at the B3LYP/6–31+G* level of theory shown for the optimized structures without Li whereby angles are shown in angles ($^{\circ}$) and bond distances in angstroms (Å). Where structures are denoted as glucose (1), fructose (2), galactose (3), mannose (4) and ribose (5).

This trend is again observed in galactose with an important dissociation energy of -4.34 kcal/mol when the metal is included, and the corresponding 3.61 kcal/mol when we consider the system without the presence of the metal.

A different behaviour to glucose, fructose and galactose is distinguished in the respective dissociation energies for the mannose system: values of 4.97 kcal/mol without metal and 4.93 kcal/mol with metal, in other words, we appreciate a dissociation energy

decrease in comparison to the presence of metal and the absence of it.

In the last system with ribose we see again a significant increase in the dissociation energies after metal exposure; 5.28 kcal/mol with metal and 2.59 kcal/mol without metal.

The general trend that we can observe in the results is that upon exposure to a metal ion the electronic affinity of the system (due to charge transfer and symmetry breaking) increases the interaction.

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