

Binding of alkyl radicals onto graphene - a DFT study

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Grafting alkyl groups onto graphene remains an open question in terms of their geometry, binding strength, the type of the created bond, and the activation energy required for such a process to occur. To further understand the grafting process, we used Density Functional Theory (DFT). A 5x5 armchair hydrogen-passivated graphene monolayer was used as a study model for this purpose (Figure 1). The surface concentration and distance between the attached alkyl groups provided critical information about their influence on the interaction strengthening caused by the cooperative actions of the first grafted group on the second [2].

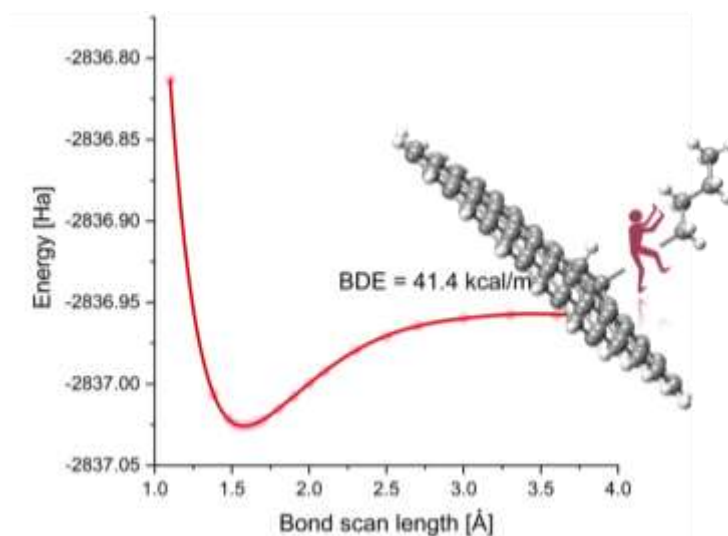


Figure 1. Bond Dissociation Energy (BDE) of the grafted graphene surface (5x5 ZigZag hydrogen passivated model).

When the bonded alkyl moieties possess functional groups, as demonstrated by Molecular Dynamics, this provides an easy way to alter graphene's dispersion properties. The Density Overlap Zones Indicator (DORI) analysis was used to visualize both covalent and noncovalent interaction regions simultaneously using a real space function. The two-dimensional electron localization function plot and three-dimensional DORI surface demonstrate unequivocally the covalent bonding between the alkyl radical and the graphene surface. The same conclusion is drawn from the computed Laplacian Bond Order (LBO), certainly proving once again the bond's covalent nature.

References

- [1] Berisha, A., Chehimi, M. M., Pinson, J. & Podvorica, F. I. Electrode Surface Modification Using Diazonium Salts. in *Electroanalytical Chemistry* 115–224 (CRC Press, 2015).