Nano porous graphene for gas purification: A quantum chemical investigation

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Abstract:

In the present study the adsorption of some gas molecule such as H_2S and CO_2 on porous graphene using first principles density functional theory calculation have been investigated. The adsorption geometries, adsorption energies, charge transfer and electronic band structures are obtained. The results of our study propose using porous graphene sheet as highly efficient and highly selective membranes for gas separations.

Introduction:

Graphene, a two dimensional sheet with sp^2 hybridized carbon atoms, is become important in the field of material science. The most application of graphene is in industry, such as gas sensor, gas purification, batteries and fuel cells. In this way porous graphene is a collection of graphene related materials with nano pores in the graphene plane. Porous graphene exhibits properties distinct from those of graphene, leading to its potential applications including energy storage, gas purification and DNA sequencing [1-3]. In this study the capability of porous graphene to separate mixture of some gases such as CO_2 and H_2S analyzed using density functional theory.

Methods:

Quantum mechanical calculations were carried out with the Gaussian program series 2009. The geometries of porous graphene (PG), CO_2, H_2S, PG/H_2S complex and PG/CO_2 complex were fully optimized employing B3LYP method with the standard 6-31G*basis set. All full optimizations were performed without any symmetry constrains.

Result and Discussion:

In the first step the absolute energy of porous graphene and gas molecules (CO_2 and H_2S) by separate geometry optimization at the same level of theory have been calculated. Figure 1(A) demonstrate of optimized geometry of porous graphene using B3LyP/6-31G*method. Table 1 shows some geometrical parameters of optimized porous graphene. In

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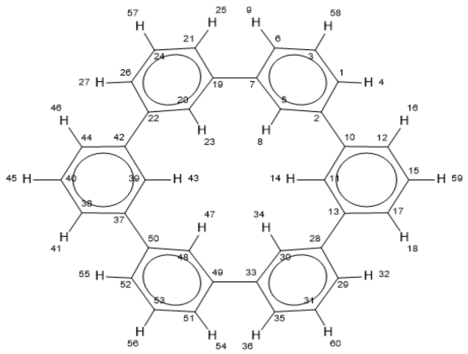
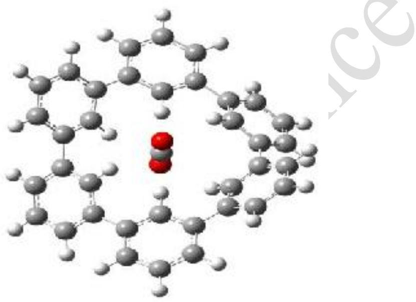
continue each single gas molecule has put in to the pores and optimize to the transition state of the system. Figure 1(B) reveals the optimized structure of CO_2 in Porous graphene. We estimate the reaction barrier for the propagation of some gas molecules through porous graphene by calculating the relative energies of the first order saddle points for systems including of a finite porous graphene plus a selected gas molecule.



(A)



(B)

Fig. 1. (A): Optimized structure of porous grapheme (B): Fully relaxed geometry of CO_2 in porous grapheme at B3LYP/6-31G* level.

Table 1. Some geometrical parameters of optimized porous grapheme.

Connected atom	Bond distance(A°)
C39-H43	1.08235
C42-C22	1.49015
C39-C37	1.40271
H43-H14	3.69214

Conclusion:

The result of our calculations reveals that porous graphene is a semiconductor with a direct band gap. Also for a porous graphene with large nano pores in the plane, the electronic conductivity could be decrease as a result of destruction of the integrity of the conjugated sp^2 carbon network. In addition porous graphene is an ideal material for gas separation and purification.

References

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