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A Possible Superstructure: Hyper Graphite

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We have shown a theoretical method to construct structures called "hyper-graphite which can be regarded as a generalization of the graphite structure. Based on the method, we propose a possible 3-dimensional network, which may be realized as a π-electron system of hydro-carbon. Naturally, localized edge states emerge at the Fermi level similar to the zigzag-edged graphite sheet.

Keywords: graphite; zero gap semiconductor; edge states; polyacene

It is well known that graphite is a semimetal and theoretically it is believed that a single sheet of graphite will become a zero-gap semiconductor. Because of very unique characters of graphite, numerous studies have been done on it. Recently, we have found that there exist lots of graphite-like structures which can be predicted theoretically. Namely, we have given a method to construct network structures being a zero-gap semiconductor having zero-energy surface (or edge) states.[1] Our method works in arbitrary dimensions. In this article, we will demonstrate that the method actually predicts a new 3-dimensional (3D) structure, which is expected to be realized as a hydro-carbon.

Our starting point is the study of graphite in nanometer scale, called "nanographite". We have revealed that zero-energy states emerging at zigzag edged graphite, namely zigzag ribbon, causes many interesting effects. [2,3,4] This localized states are called "edge states". Edge states give a sharp peak at Fermi level in density of states (DOS). Orbital magnetism and localized magnetism of the graphite ribbon are deeply affected by the edge states.[2,4]

Now, an important step to find a generalization of graphite is reconsideration of our analytic solution of edge states.[1] The solution suggests a way "to create a structure" having similar zero-energy states as the graphite zigzag ribbon. We can actually construct a network structure iteratively so that edge states are an eigen state. We call these structures made by this method "Hypergraphite"[4]. This is because structures have both characters of topology and electronic states of the 2D graphite sheet.

We explain the method to make N-dimensional hypergraphite. The method is summarized as following steps. i) Prepare a $(N-1)$-dimensional AB bipartite structure on which at least one non-bonding orbital (NBO) having amplitude only on A-sites exists. ii) Put copies of this structure side by side from the origin to N-th direction. Here, we number structures $(i = 1, 2, \cdots, \infty)$ successively. iii) Connect B-sites of i-th structure with A-sites of $(i+1)$-th structure by extra bonds. Utilizing this method, we obtain a N-dimensional AB bipartite structure on which non-bonding edge states exist. Details of conditions to be hypergraphite is given elsewhere.[1]

We show an example of 3D hypergraphite in FIGURE 1-(a). This 3D three-coordinated structure (we call it H1) is made of 2-D bipartite structures shown in FIGURE 1-(b). Naturally, we can construct NBOs on this structure.

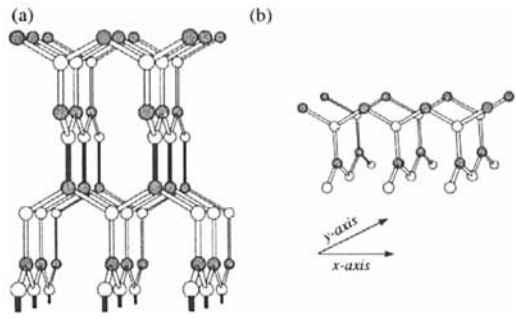

FIGURE 1. (a) A 3-dimensional three-coordinated structure (H1 structure). (b) A 2-dimensional bipartite structure which is made by combining zigzag chains aligned in x-axis and zigzag chains aligned in y-axis. This is a building block of H1.

To discuss electronic state on H1, we consider a tight-binding model,

where each site has only one s-like wavefunciton and transfer integrals are equal to unit between connected sites. On-site energy is equal to zero. A band structure of a slab model of H1 as well as the 1st Brillouin zone (1st BZ) are shown in FIGURE 2. We recognize that there are two almost flat bands around Fermi level. This is an evidence that edge states emerge on this structure.

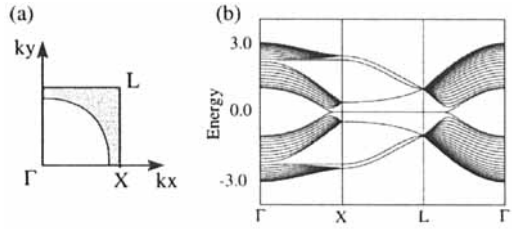

FIGURE 2. (a) A 1st Brillouin zone of H1structure. Edge states emerge in the shadowed space. (b) A band structure of slab model of H1 structure. This structure is made by connecting ten blocks shown in FIGURE 1-(b).

H1 structure is actually found as a network of Si atoms in α-$ThSi_2$ structure. However, we cannot apply the above simple s-band model to discuss real materials. So, we now proceed to predict another structure, which is expected to be realized as a carbon network.

We show an example of realistic hypergraphite giving a π-electron network in FIGURE 3-(a). All two connected sites are assumed to be terminated by hydrogen. This network can be regarded as a superstructure made of polyacene. Thus we call this π-electron network "Hyper Polyacene" (HP). The important point is, however, that this structure is created by the method to make a hypergraphite, so that the electronic state should possess characters of hypergraphite.

We calculate a band structure of slab model of HP with zigzag edge. This calculation is based on a tight binding model that consists of $2s$, $2p$ orbitals of carbon atoms and $1s$ orbitals of hydrogen atoms as basis functions. We use a parameter set which is made by M. D. Winn *et al*[5]. As shown in FIGURE 3-(c) and (d), these are two almost flat bands around Fermi level in the band structure. We can also obtain an analytic expression of this edge states in π-electron network of this structure. From these

facts, we can say that a hypergraphite with π-electron system is possible. If this hydro-carbon is made, it will show interesting properties coming from edge states.

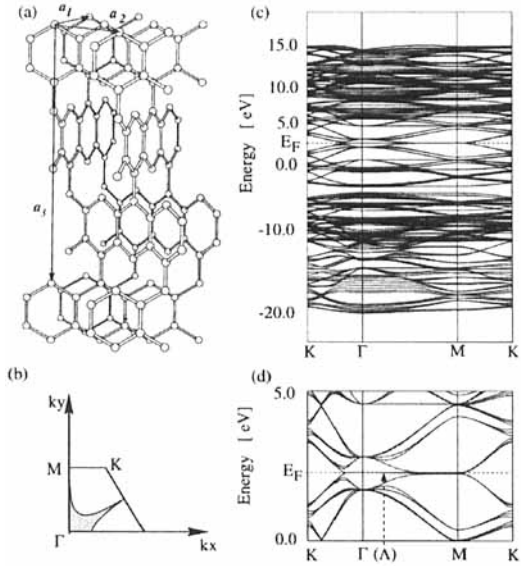

FIGURE 3. (a) A Skeleton of Hyper Polyacene (HP). a_1, a_2 and a_3, are primitive translation vectors. All two connected sites are assumed to be terminated by a hydrogen. (b) The 1st Brillouin zone of a slab model of HP with zigzag edge. Edge states emerge in the shadowed space. (c) A band structure of slab model of HP with zigzag edge. (Λ) indicates two flat bands which are made from edge states. Bands around the Fermi level are magnified in (d).

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