P847 Quantum Chemical Study of Sodium Intercalation to Graphene Sandwich Structure

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Unlike lithium, sodium cannot be intercalated between graphite layers, so that the sodium ion battery with a graphite negative electrode has been considered impossible. On the other hand, in 1983 and in 1987, we found that the polyacenic semiconductor (PAS) as a kind of hard carbon occluded sodium and lithium respectively(Table1), and worked effectively as an electrode in an organic electrolyte cell [1,2].

Table 1. The electrical conductivity (σ in S/cm) and dopant concentration

	pristine	Na-doped [1]		Li- doped[2]	
sample	σ	σ	[Na]/ [C]	σ	[Li]/ [C]
D	8.5×10^{-6}	3.5×10^{-1}	0.058	3.5×10^{-1}	0.016
E	1.2×10^{-1}	2.9×10	0.058	4.7×10^{0}	0.016
G	2.7×10	4.5×10	0.066	8.2×10	0.037

In this study, sodium intercalation to the graphene sandwich structure is investigated by quantum chemical methods to explore the occluding of sodium atoms to non-graphitizable or hard carbon. We found that the C_8Na composition was energetically preferable to the C_6Na composition(Figure 1). For the sodium intercalation, the space between the sheets extended from the graphitic one (3.4 Å) to 4.6 Å, larger than that for the lithium intercalation by 3.9 Å. The net charge of the intercalated sodium was around 0.82; the sodium atoms were more strongly ionized than the lithium atoms by the intercalation. Occluding of sodium atoms to hard carbon materials depends on the size of the graphene sheet as well as on the structure of the surface.

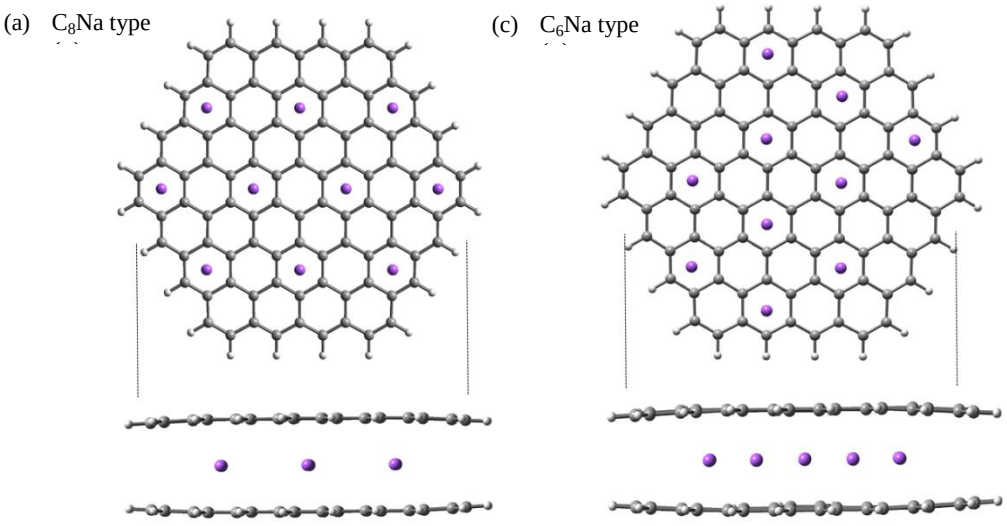

Figure 1. The optimized structure of a pair of $C_{96}H_{24}$ occluding ten Na atoms. The structures (a) and (b) represent the C_8Na and C_6Na compositions in the bulk state, respectively.

References:

[1] T. Yamabe, et al., J. Phys. Colloques, 44(1983) C3–645.
[2] T. Yamabe, et al., Syn. Met., 18, 515 (1987).