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Computational Chemistry Approach to Investigate the Electrical Properties of Carbon Black

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【Introduction】

Carbon black finds wide range of application such as in electrodes of fuel cells, as conductive packaging for electronic components etc. due to their unique electrical properties. The unique electrical properties of carbon blacks are rendered by the organic functional groups attached in the periphery or the in plane defects on the basic structural units of the carbon black. Where, the basic structural units in carbon black constitutes of graphene layers that are concentrically oriented[1)]. In the present study computational chemistry approach have been employed to investigate into the relationship of electrical conductivity of carbon black and its chemical topology.

【Method】

In the present study a novel program, Colors, based on tight-binding quantum chemical method has been employed to investigate the electrical properties of carbon black. In this work Colors program combined with Drude model and Monte Carlo method has been employed to estimate the electrical conductivity[2)]. DMol[3] another program based on DFT has been also used to investigate the electronic properties of carbon black. All the calculations by DMol[3] were performed at DNP level of basis set and GGA/PW91 exchange and correlation functional.

【Results and Discussion】

Prior to the investigation on the electrical properties of carbon black a study on the electrical properties of graphite was investigated as a validation of our methodology for its application to understand the electrical properties of different kinds of carbon materials. This work on graphite revealed that the electrical conductivity of graphite along the plane parallel to the basal plane ($\sigma_{\parallel}$) is 0.7×10^4 S cm^{-1} and the electrical conductivity of graphite along the plane parallel to the basal plane is ~10^3 greater than plane perpendicular ($\sigma_{\perp}$) to it (Table I). These observations agree with the former experimental observations. Investigations on the electrical properties of carbon black were then carried out. It was observed that electrical conductivity of carbon black models increased considerably with the increase in sulfur containing groups see (Table 2). This increase in electrical conductivity of carbon black models with increasing sulfur-containing groups is probably due to the increasing contribution of S 2p orbitals in the highest occupied molecular orbital. The electrical conductivity of all the models was found in the experimental range. In this investigation it was further revealed that the electrical conductivity of carbon black is inversely related to the ratio of carbon atoms in the periphery of the basic structural units to the carbon atoms only attached to the carbon atoms in the basic structural units. Thus, it was theoretically observed that the electrical conductivity of carbon black is dependent on several factors such as size, functional groups attached to the basic structural units and their conformational arrangements.

Table I. Electrical conductivity of graphite

System	Electrical conductivity (S cm^{-1})					
	$\sigma_{\parallel}$		$\sigma_{\perp}$		$\sigma_{\parallel}/\sigma_{\perp}$	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp
Graphite	7.0×10^4	$(2.6\pm0.2)\times 10^4$	1.6×10	150-230 (± 20%)	4.4×10^3	10^2- 10^3

Table II. Electrical conductivity of carbon black with increasing –SH groups and decreasing –OH groups

System	Electrical conductivity (S cm^{-1})	
	Calc.	Exp.
$CB(OH)_2(SH)$	2.8	2.5-4.7
$CB(OH)(SH)_2$	3.1	
$CB(OH)(SH)_3$	4.7	

【References】

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