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Theoretical investigation on the electronic and electrical properties of carbon materials

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【Introduction】

With the pioneering works on the conducting polymers in mid-seventies there has been a tremendous increase in the research on the electrical properties of polymers undertaken by both theoreticians and experimentalists equally. However, most of the theoretical works on this field are focused on understanding the optical and electronic properties of polymers e.g., Weimer[1] et al., have shown the effect of chain length on the energy gap of polymer chain. In the present work we focus our studies to understand not only the electronic properties but also the electrical properties of doped and undoped polyacetylenes with the general formula C_nH_{n+2} [n = 2, 4, 8, 10, 12 and 16].

【Method】

Colors - a program based on tight-binding quantum chemical molecular dynamics was used in this work for studying the electronic properties and estimating the electrical conductivity. The electrical conductivity was estimated by using Drude's model i.e., $\sigma=ne\mu$, where σ, n, e and μ stands for electrical conductivity, number of carriers, elementary electrical charge, and mobility respectively. In our studies the fully optimized structures were used. The structures were optimized using DMol[3], at DNP level of basis set with GGA/PW91 exchange and correlation functionals. CASTEP program was also used for discussing the electronic structure of systems under investigation.

【Results and Discussion】

In this work preliminary investigations on electronic and electrical properties of diamond and graphite were performed. Table 1 summarizes the results obtained from this investigation. The good agreement of the calculated values for band gaps of diamond and graphite and the electrical conductivity of graphite with the experimental values validated our methodology for its application to study the electronic and electrical properties of carbon materials. We then carried our studies on the electronic and electrical properties of linear polyacetylene chains. From our studies we observed that HOMO-LUMO energy gap decreases with the increase in the carbon chain length while the electrical conductivity increases. The energy gap obtained from the Colors for all the systems were in good agreement with the experimental findings[2]. This study was then extended to the study of polyacetylene doped with bromine. In this study we further observed that the doping of polyacetylene systems with bromine increased the electrical conductivity by an order of ~10^{-9} (Table 2). This observation is in good agreement with the experimental findings. In this presentation a detailed discussion on the electronic and electrical properties of these carbon mateirals shall be presented.

Table 1 Theoretically estimated energy gap and electrical conductivity of diamond and graphite

System	Energy gap (eV)		Electrical conductivity Scm^{-1}	
	Calc.	Exp.	Calc.	Exp.
Diamond	5.6	5.5	$5.6x10^{-32}$	~10^{-13}
Graphite	0.0	0.0	$0.7x10^{5}$	~10^{5}

Table 2 The HOMO-LUMO energy gap and electrical conductivity of C_8H_{10}, C_8H_9Br and $C_8H_{10}Br_2$

System	HOMO-LUMO energy gap (eV)		Electrical conductivity (Scm^{-1})
	Calc.	Exp	Calc*.
C_8H_{10}	4.57	4.4	$1.0x10^{-5}$
C_8H_9Br	3.39	-	$0.8\ x10^{4}$
$C_8H_{10}Br_2$	3.48	-	$2.7x10^{4}$

*Normalized using experimental values

References:

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