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# Investigation on Electrical Properties of Carbon Black by Ultra Accelerated Quantum Chemical Molecular Dynamics

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## 【Introduction】

The electrical conductivity in carbon blacks is strongly dependent on the structure, specific surface area, particle size, separation distances of the particles etc. It has been also reported that different forms of carbon blacks have different electrical conductivity in spite of their similar structure. This difference in electrical conductivity might be associated with the chemical topology of the carbon black. In the present investigation an ultra accelerated quantum chemical molecular dynamics program (UAQCMD) has been employed to investigate realistic carbon black models.

## 【Method】

Recently, we have developed UAQCMD program by combining tight-binging (TB) and classical molecular dynamics (MD) method. This method is ten million times faster than other first principle methods. In this method the two, three and four body potentials obtained from TB calculations are used to perform MD simulations. 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/PBE exchange and correlation functional.

## 【Results and Discussion】

First UAQCMD calculations were performed on graphite structure. It was seen that after the UAQCMD calculations electronic properties of graphite such as energy gap is found to be in good agreement with the experimentally determined value of 0.0 eV. The calculated binding energy and bond population of bonding and non-bonding atoms are also seen to be comparable with DFT calculations. This validated the reliability of the newly derived TB potential parameters for MD simulation to study related carbon materials. In the next step realistic models of carbon blacks were constructed Fig. 1. The calculated densities of carbon black are 1.11 g/cm$^3$ and 1.64 g/cm$^3$. From this investigation it was seen (Table I.) that the electrical conductivity of carbon black are enhanced by increase in density of the carbon black models. This increase in electrical conductivity can be attributed to the increase in the electrical contacts between the basic structural units [1]. The calculated electrical conductivity is in the range of experimentally reported values. This study is further extended to understand the electrical properties of carbon black with and without sulfur contents.

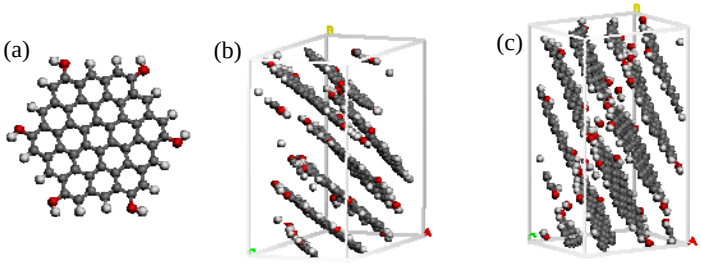


Fig. 1. (a) Basic structural unit of carbon black models and realistic carbon black models with density of (b) 1.11 g/cm$^3$ and (c) 1.64 g/cm$^3$

Table I. Calculated and experimental density and electrical conductivity of carbon black models

| System | Density | | Electrical conductivity (S/cm) | |
|---|---|---|---|---|
| | Calc. | Exp. | Calc. | Exp. |
| CB | 1.11<br>1.64 | 0.34~1.80 | 3.541<br>5.533 | 0.20~100 |

## 【Reference】

[1] J. Sanchez-Gonzalez, A. Macias-Garcia, M. F. Alexandre-Franco, V. Gomez-Serrano, *Carbon* **43** (2005) 741.