**Energetics of Lithium Ion Diffusion in Defective Carbon Nanotube**

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Rechargeable lithium ion batteries have been widely used as the compact power sources for information technology devices. The charging and discharging process in these batteries is controlled by exchanging lithium ions between the negative and the positive electrodes through the separator. The expected features of electrode materials are; (1) large electronic capacity, (2) good reversibility, (3) quickness for the charging process, and (4) environment-friendly characteristics, while serving the economical issues. The metallic state of lithium is not suitable for negative electrode material due to the explosive property. It has been suggested, both experimentally and theoretically, that the carbon nanotube is one of the promising candidates for the negative electrode material of high energy–density while overcoming the difficulties.[1, 2]

In the present work, the lithium ion diffusion in the single walled carbon nanotube (SWNT) was systematically studied by using the density-functional total energy calculation. We first studied the (5,5) SWNT systems having the intrinsic $n$ ($n$ , 7) □ membered carbon–ring defects. The calculated defect formation energies of the $n$ = 7, 8, and 9 membered carbon–ring defects (Heptagon, Octagon, and Enneagon rings) were 3.9 eV, 7.09 eV, and 10.07 eV, respectively. We next investigated the energetics of diffusion pathways for lithium ion to move through the center of defective rings (Figure 1). We find strong unsymmetric energetic variation with respect to the center of ring (point B) in the case of the $n$ = 9 (Enneagon ring), where the energy minimum outside the tube is about

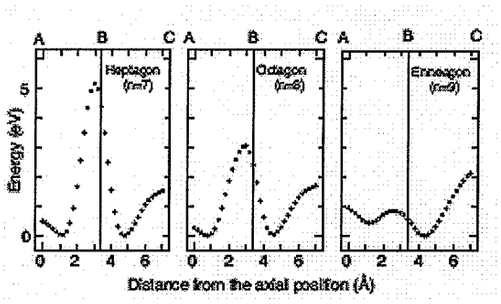


Figure 1: Energetics of diffusion pathways for lithium to move through the center of defective rings (point B) of the (5,5) SWNT. The point A shows the position on the center axis and C the position outside the SWNT such that B is the mid-point between A and C. Energy is measured relative to the most stable value.

0.5 eV lower than that of the interior. Our results for the defect formation energies and the diffusion barriers are somewhat different from those of Meunier *et al.*[2] More detailed diffusion dynamics and potential applications will be discussed.

This work was supported by the Grantin-Aid for Scientific Research from the Japanese government. The authors thank the Supercomputer Center, ISSP, University of Tokyo for providing us with the computing facilities.

**References**

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[2] V. Meunier *et al.*, Phys. Rev. Lett. 88, 75506 (2002).