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Computer Simulations for a Novel Topological Defect on Carbon Nanotube TAKAZUMI KAWAI, Fundamental and Environmental Research Lab., NEC Corp., SUSUMU OKADA, Inst. of Physics and Center for Computational Sciences, Univ. of Tsukuba, KEI KUWABARA, KOTA DAIGOKU, KYOKO NAKADA, Dept. of Chemistry and Biological Science, Aoyama Gakuin Univ., YOSHIYUKI MIYAMOTO, Fundamental and Environmental Research Lab., NEC Corp. — Topological defects in carbon nanotubes do not just causes a nuisance to the nanotube devices, but they sometimes provide new and interesting properties to them. Since the defect physics of nanotube is just in the early stage of research, it is very important to verify the stability and electronic properties of such defects theoretically prior to experiments. Here, we performed TBMD simulations for defect formations by C_2 molecule irradiation. Although C_2 molecule often bounce back even with a high kinetic energy of $\sim$20 eV, it irradiates several famous defects such as mono-vacancy, di- vacancy, and also Stone-Wales defect. In similar simulations, we also found a novel defect structure, where C_2 molecule is incorporated into sp^2 network of nanotube. Thermal stability of the nanotubes with the defects is similar to that of intact ones. Interestingly, DFT-LSDA calculations showed that nanotubes with a line of the novel topological defects are found to cause a magnetic ordering, where the polarized electron spins are localized around the defect and ferromagnetically aligned along the tube axis. This work was in part performed under the management of Nano Carbon Technology project supported by NEDO.

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