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Ab initio **study of novel carbon nanofoam structure as an anode material for Li secondary battery** HANJIN PARK, SORA PARK, SEOUNG-HUN KANG, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University — Using ab inito density functional theory, we investigate the adsorption and diffusion properties of Li atoms on a new carbon nanostructure, which may be used as an anode of Li secondary battery. We focus on a special carbon nanofoam structure consisting of Schwarzite structures with negative Gaussian curvature as core parts, which are interconnected through (4,4) CNT segments. Considering the symmetry of the nanofoam structure, we find various Li adsorption sites exhibiting relatively large binding energies ($\gtrsim$2.00 eV). Based on these adsorption sites, we identify several diffusion paths on the outside or inside surface of the nanofoam structure and examine the diffusion barriers along the paths. Our results show that Li atom can diffuse almost freely due to its low energy barriers on both outside and inside surfaces. Finally, we also evaluate the energy gain tendency and the volume expansion as well as the average binding energy while adding Li atoms to estimate the Li-capacity and recyclability of the system, which are important characterisitics for anode materials. We conclude that the carbon nanofoam structure would be better as an anode material than graphite in Li capacity and volume expansion.

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