

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Multilayer Graphynes for Lithium Ion Battery Anode HOONKYUNG LEE, Konkuk University — Graphynes, two-dimensional layers of *sp*- and *sp*²-bonded carbon atoms, have recently received considerable attention because of their potential as new Dirac materials. Here, focusing on their large surface area, we explore the applicability of graphynes as lithium ion battery anodes through the first-principles density functional calculations. We have found that Li potential energies are in the range suitable to be used as anodes. Furthermore, the maximum composite of Li-intercalated multilayer α - and γ -graphynes is found to be C₆Li₃, which corresponds to a specific capacity of 1117 mAh g⁻¹, twice as large as the previous theoretical prediction for graphynes. The volumetric capacity of Li-intercalated multilayer α - and γ -graphynes is 1364 and 1589 mAh cm⁻³, respectively. Both specific and volumetric capacities of Li-intercalated graphynes are significantly larger than the corresponding value of graphite, from which we conclude that multilayer graphynes can serve as high-capacity lithium ion battery anodes.

Hoonkyung Lee
Konkuk University

Date submitted: 21 Nov 2012

Electronic form version 1.4