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Alkali Metal Intercalation in Curved Carbon Networks: X-Ray Structural Studies

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The intercalation of alkali metal ions into carbon-based aromatic systems is of great interest in materials science due to the increased need for stable anode materials with high capacity of energy storage. Currently, graphite, a sp²-hybirdized carbon network, is the key anode component in rechargeable Li-ion batteries. Carbon allotropes with nonplanar π -surfaces, ranging from fullerenes to nanotubes, are now under investigation as prospective anode materials. The curved carbon networks of fullerenes and nanotubes are often modeled by open bowl-shaped polyaromatic hydrocarbons, such as the smallest curved fullerene fragment, corannulene (C₂₀H₁₀). One of the most fascinating properties of such bowl-shaped polyarenes and fullerenes is their ability to reversibly uptake and delocalize extra electrons upon multi-electron reduction without significant rearrangement and deformation of their carbon framework [1,2]. Notably, the anode material fabricated from corannulene shows a high reversible lithium capacity (602 mAh/g). This is almost twice as high as the theoretical capacity of the commonly used fully lithiated planar graphite material (LiC₆, 372 mAh/g). In our work, we target the X-ray structural elucidation of metal intercalation patterns of carbon-rich curved polyarenes with light alkali metal ions, such as Li and Na, and compare those with extended planar polyaromatic systems. Recently, we expanded this study to the light alkaline earth metal, Mg, as its atomic radius is very close to that of Li. In addition, magnesium is cost effective and abundant, and thus presents great interest in the emerging energy storage technologies.

[1] A. V. Zabula, A. S. Filatov, S. N. Spisak, et al., *Science*, 2011, 333, 1008–1011., [2] S. N. Spisak, N. J. Sumner, A. V. Zabula, et al., *Organometallics*, 2013, 32, 3773–3779.

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