**Enabling carbon nitride materials as lithium ion battery anode materials through fundamental understanding**

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Carbon structures have been extensively studied over recent decades as energy storage materials. One of the industry applications is as the anode of lithium (Li) ion batteries (LIBs). Graphite, a layered material consisting of sp2 bonded carbon sheets, is currently the predominant anode material offering a theoretical capacity of LiC6 with Li inserted between the layers.

Doping carbon materials with nitrogen has been shown to increase the storage capacity if used as an anode material. Graphitic C3N4 is a well-known and widely used material with a high nitrogen content. However, it is not suitable as a LIB anode material, as its interaction with lithium is too strong so that the lithium cannot be discharged again.

We have performed comprehensive studies of a range of carbon nitride materials to understand the mechanism of the interaction of the lithium with the carbon nitride material. We have modified graphitic C3N4, by breaking it into ribbon like structures and combining it with a carbon backbone, to increase its reversible storage capacity and to provide a path to harness carbon nitrides as lithium ion anode materials.

Density functional theory (DFT) calculations are employed to obtain the maximum lithium storage capacity. We also calculate diffusion barriers for the lithium movement from one site to another to determine their mobility. In addition to this we also show how the lithium binds to the material by consideration of the charge density distribution and the charge transfer from the lithium to and from the material. The volume change of the material on the insertion of lithium is determined by employing a bilayer or bulk configuration of the material. Our calculations are combined with experimental investigations. These interdisciplinary studies confirm that modified carbon nitrides could be suitability as LIB anode materials. They show that combining experiment with the fundamental understanding of calculations can provide a pathway to designing new LIB anode materials.