Pair distribution function analysis of hard carbon anode materials for sodium-ion batteries.

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Sodium-ion batteries (NIBs) have attracted attention in recent years because of the high natural abundance of sodium compared to lithium. This makes NIBs particularly attractive in applications such as large-scale grid storage where low cost and sustainability, rather than energy density is the key requirement. Several materials have been suggested as cathodes but far fewer studies have been done on anode materials and, because of the inability of sodium to intercalate into graphite, the anode material of choice in commercial lithium-ion batteries, the anode represents a significant challenge to this technology. Hard carbons have been demonstrated to have a high capacity for sodium. However, the lack of crystallinity displayed by these materials makes them challenging to characterise. Here, pair distribution function (PDF) analysis - a total scattering technique which is sensitive to local structure - has been used to gain information about the structure of hard carbon anodes. Operando PDF experiments, combined with solid-state nuclear magnetic resonance, are able elucidate details about the sodium-storage mechanisms in hard carbon anode materials, and make links between the local structure and electrochemical properties in different hard carbon materials. Our results indicate that the capacity results from sodium ions first adsorbing onto pore surfaces, defects and between expanded layers, before pooling into larger, quasi-metallic clusters or between expanded carbon sheets at lower voltages.