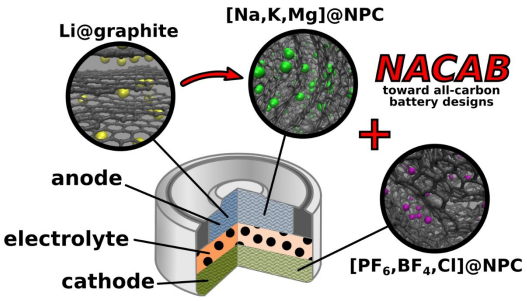

NACAB

Nanocellulose-derived hard carbons for sustainable Na-ion anodes: an experimental and computational study.

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Li-ion batteries are not a sustainable energy storage solution. Lithium is a scarce resource and difficult to recycle. However, intercalants that can be produced sustainably, such as Na, cannot readily intercalate into the standard graphitic anodes used in traditional Li-ion batteries. Porous carbon anodes produced from nanocellulose pyrolysis provide a promising alternative, having an atomistic structure that could accommodate larger ions. We synthesize and assess the potential of different nanocellulose derived hard carbon anodes for use in Na-ion batteries and investigate their performance and structure using experimental and computational techniques. Characterization was performed by XRD, Raman, XPS, SEM and HRTEM showing significant deviations in electrode structure with different nanocellulose precursors. Bacterial nanocellulose electrodes were shown to give the best electrochemical performance which correlated with cumulative pore size and C=O content, implying exemplary Na intercalation and adsorption behavior. We elucidate the atomistic structure of these amorphous carbon electrodes by performing novel simulations combining the XRD data with Machine-Learned Potentials to generate experimentally valid anode structures to gain insights into their different characteristics. We further show the effect of Na intercalation on cell expansion in amorphous and graphitic carbon. This work demonstrates the capability of nanocellulose derived anodes as a new, viable material for use in Na-ion batteries, providing a solution for sustainable energy storage. In addition, we show that experimental data can be combined with simulation to gain experiment-specific insights into the atomistic structure and the potential mechanisms at play in these systems.

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I will present experimental results of electrochemical performance of various nanocellulose anodes, experimentally valid atomistic structures from the novel simulation protocol and show the effect of ion intercalation in amorphous carbon and graphite.