Multiscale Mechanical Modeling of Polysaccharide-Derived Aerogels for Energy-Storage Devices

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Chitosan-based aerogels are promising sustainable materials for energy storage and lightweight structural applications, due to their high porosity, low density, and tunable pore architecture. However, their performance in practical devices - particularly in battery electrodes - depends critically on mechanical stability during processing and operation, where granular assemblies are subjected to compressive stresses that can induce pore collapse, particle rearrangement and affect porosity, permeability and electrical percolation. Following these challenges, a multiscale simulation framework was developed, combining a bonded-particle discrete element method (BPM-DEM) with a resistor network model (RNM). The BPM-DEM model captures interparticle forces, contact mechanics, and microstructural evolution under compression, validated against experimental uniaxial loading data of chitosan and carbone aerogels. The resistor network model is embedded within the same microstructural representation to quantify how mechanical deformation - such as contact, particle displacement, and pore collapse - affects electrical conductivity. This integrated approach reveals that the electrical performance of granular aerogel electrodes is highly sensitive to powder and pore architecture. The framework enables predictive design of chitosan aerogels for functional applications, providing quantitative guidance for achieving robust, conductive, and processable electrode architectures.

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