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

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Polysaccharide aerogels (e.g., cellulose, chitosan) are attractive, lightweight, high-porosity materials for energy storage, filtration, and thermal insulation. When carbonized, polysaccharide aerogels evolve into porous carbon materials that are especially promising as electrodes for lithium-ion, sodium-ion and solid-state batteries. Understanding their mechanical behaviour from the microscopic pore network to the macroscopic powder is essential to guarantee structural integrity during processing, assembly, and cycling.

A universal, multiscale simulation framework based on the Discrete Element Method (DEM) extended with a bonded-particle model (BPM), capturing both inter-particle forces and bonds representing polymer networks, has been developed. The modelling approach is validated against bulk compression experiments for aerogel samples, allowing realistic prediction of elastic regime, progressive pore collapse and network densification. Polysaccharide-derived carbon aerogels are modeled by modifying the bond stiffness, mimicking the reduced polymeric bonding and mass loss after carbonization, while retaining the same micro-geometric representation.

The framework is further applied to granular assemblies of aerogel particles to study how contact mechanics, bond yielding and breakage affect their mechanical response and structural integrity, which are key factors in electrode slumping and current-collector adhesion in battery stacks. The DEM-based analysis demonstrates that, for battery-grade carbon aerogels, the mechanical stability of the electrode can be optimized by tailoring the pore size distribution and powder particle size, thereby balancing ionic transport and mechanical robustness.

The results highlight the power of the bonded-particle DEM in bridging scales, from nanoscale pore networks to bulk powders, providing quantitative guidance for the rational design of polysaccharide-derived aerogels for next-generation energy devices.

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