Energy Conversion in Polyelectrolyte Hydrogels

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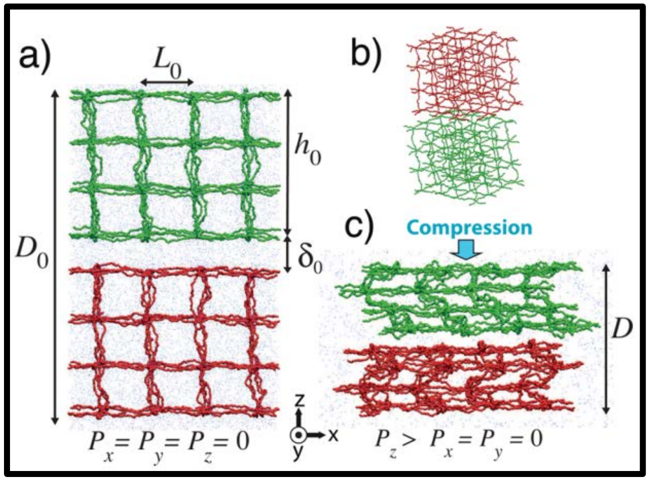

Figure 1. Illustration of compression simulations of a double hydrogel system of identical gels with a charge fraction f = 0.5 and polymerization degree N = 128. Counterions are rendered as dots. (a) Underformed hydrogel slabs separated initially by a gap of thickness δ_0, (b) 3D view of the hydrogels, and (c) uniaxially compressed gels. Note that the dangling ends at the edges are bonded to those in the adjacent periodic gel. In the actual simulations, $\delta_0 \approx h_0$. All snapshots are obtained via VMD.

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Work was performed at Northwestern University.

Scientific Achievement

Molecular dynamics (MD) simulations demonstrate that upon deformation, hydrogels adjust their deformed state predominantly by altering their electrostatic interactions.

Significance and Impact

The ability to adjust their internal electrostatic interactions in response to electromagnetic fields or mechanical deformations make hydrogels ideal candidates for energy converters and actuators.

Research Details

– A double gel system was designed in which two semi-infinite hydrogel slabs are separated by a large polymer-free region, to which counterions can escape, as shown in Figure 1.

– The relationship between deformation and energetic changes in PE hydrogels was investigated by means of MD simulations.

– Electroneutrality conditions inside the gel cause the charged backbone groups and counterions to rearrange themselves to reduce the total electrostatic energy and form ionic structures.

– Counterions remain in the gel even under strong compression resulting in significant alteration of the electrostatic energy.