Simulating the Swelling of Weak Polyelectrolyte Hydrogels

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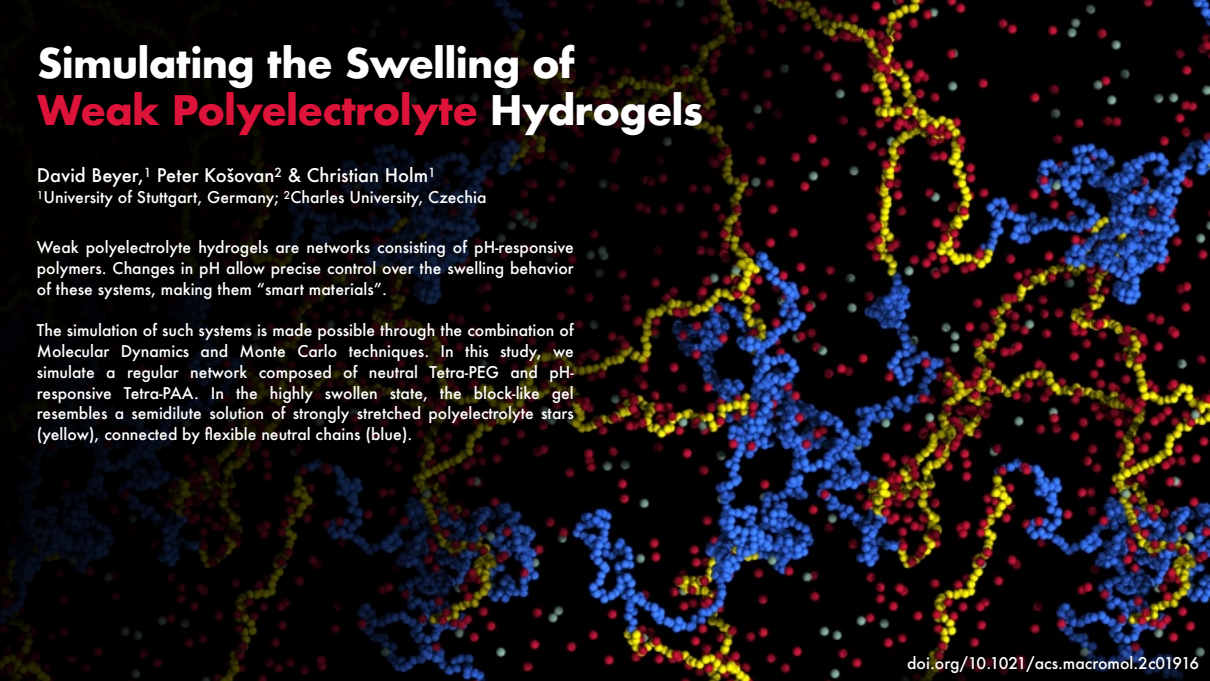
Weak polyelectrolyte hydrogels are networks consisting of pH-responsive polymers. Changes in pH allow precise control over the swelling behavior of these systems, making them “smart materials”.

The simulation of such systems is made possible through the combination of Molecular Dynamics and Monte Carlo techniques. In this study, we simulate a regular network composed of neutral Tetra-PEG and pH-responsive Tetra-PAA. In the highly swollen state, the block-like gel resembles a semidilute solution of strongly stretched polyelectrolyte stars (yellow), connected by flexible neutral chains (blue).



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