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Energy conversion in polyelectrolyte hydrogels[1] MONICA OLVERA DE LA CRUZ, AYKUT ERBAS, Northwestern University, OLVERA DE LA CRUZ TEAM — Energy conversion and storage have been an active field of research in nanotechnology parallel to recent interests towards renewable energy. Polyelectrolyte (PE) hydrogels have attracted considerable attention in this field due to their mechanical flexibility and stimuli-responsive properties. Ideally, when a hydrogel is deformed, applied mechanical work can be converted into electrostatic, elastic and steric-interaction energies. In this talk, we discuss the results of our extensive molecular dynamics simulations of PE hydrogels. We demonstrate that, on deformation, hydrogels adjust their deformed state predominantly by altering electrostatic interactions between their charged groups rather than excluded-volume and bond energies. This is due to the hydrogel's inherent tendency to preserve electro-neutrality in its interior, in combination with correlations imposed by backbone charges. Our findings are valid for a wide range of compression ratios and ionic strengths. The electrostatic-energy alterations that we observe in our MD simulations may induce pH or redox-potential changes inside the hydrogels. The resulting energetic difference can be harvested, for instance, analogously to a Carnot engine, or facilitated for sensor applications.

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