

# Adsorption of reactants on a PNIPAM polymer

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Thermoresponsive hydrogels, such as Poly(N-isopropylacrylamide) (PNIPAM), are recently becoming very popular as ‘smart’ carriers in modern nanoscience. By changing the temperature, the PNIPAM hydrogel structure can undergo a sharp transition from a swollen into a collapsed state, which alters the selectivity for the solute particles that diffuse through the hydrogel. Catalytic model reactions of the reduction of p-nitrophenol and nitrobenzene nicely demonstrate such a selectivity [1], where the reaction rates of both reactants dramatically change after the transition. In order to gain insights into the nanoscale structure, binding kinetics, and diffusion in such systems, we employ Molecular Dynamics simulations of PNIPAM polymer in explicit water. We model an extended PNIPAM polymer chain in the presence of various solutes dissolved in water, which mimics the hydrogel in the swollen state. We put particular attention on benzene and its derivatives and explore the influence of temperature, polymer stretch, and polymer tacticity on the solute binding affinities.

[1] Shuang Wu, Joachim Dzubiella, Julian Kaiser, Markus Drechsler, Xuhong Guo, Matthias Ballauff, and Yan Lu, *Angew. Chem. Int. Ed.* 51, 2229 (2012).