Rational design of stimuli-responsive nanoreactors

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The catalysis by metal nanoparticles is one of the fastest growing fields in nanoscience. However, the optimal control of catalytic activity and selectivity in nanoparticle catalysis remains a grand scientific challenge. Here, we describe our ongoing efforts how to theoretically derive design rules for the optimization of nanoparticle catalysis (in the fluid phase) by means of thermosensitive yolk-shell and core-shell carrier systems [1-3]. In the latter, nanoparticles are stabilized in solution by an encapsulating, thermosensitive hydrogel shell. The latter contains and shelters the reaction. The physicochemical properties of this polymeric 'nanogate' react to stimuli in the environment and thus permit the reactant fluxes and with that the catalytic reaction to be switched and tuned, e.g., by the temperature [1-3], salt concentration, or solvent composition. Hence, the novel hybrid character of these emerging 'nanoreactors' opens up unprecedented ways for the control of nanocatalysis due to new designable degrees of freedom, if theoretical understanding and rational design principles are available.

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