Description of catalytic rates in stimuli-responsive nanoreactors

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In recent years, the use of stimuli-responsive polymer coatings has come out as a possible new way to control the catalytic activity of colloids and nanoparticles [1,2]. The polymer coating not only prevents particles from coagulation or aggregation, but actively participates in the catalytic process by changing the local environment for the reactants. The catalytic rate can be thus flexibly tuned and switched, e.g., by the temperature [1,2], ionic strength, or pH.

In this work we present a comprehensive theoretical framework that, by extending concepts from the Debye-Smoluchowski theory of diffusion [2,3], allows to qualitatively and quantitatively describe the influence of all major experimentally tunable parameters on the nanoreactors’ catalytic rate. We pay special attention to the case of multicomponent systems by analyzing the temporal and spatial distribution of reactants and products. Besides, we study the effect of electrostatic interactions on the catalytic rate. This theoretical framework is also useful to find out what parameters most sensitively tune such rate, therefore providing theory-guided design principle for stimuli-responsive nanoreactors’ synthesis.