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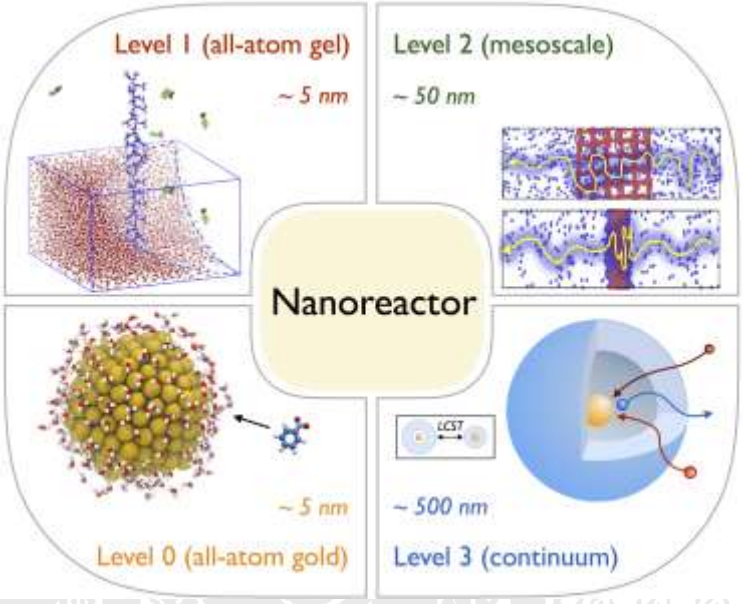

Multiscale modeling of soft functional materials: stimuli-responsive nanoreactors

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After a short introduction and overview of my general research directions, I will focus on one of my key topics, namely the investigation of so-called 'responsive nanoreactors' by computer simulations and statistical physics approaches. In these nanoreactors [1-5], metal nanoparticles are stabilized in aqueous solution by an encapsulating, thermosensitive hydrogel shell, containing and sheltering the chemical reaction catalyzed by the nanoparticles. The physicochemical properties of the polymeric hydrogel 'gate' respond to stimuli in the environment, permitting the reactant fluxes and the catalytic reaction to be switched and tuned, e.g., by the temperature, salt concentration, or solvent composition. Hence, the novel hybrid character of these emerging nanoreactors opens up unprecedented ways for the control of nanocatalysis and its adaption to the local environment by 'intelligent' response and/or internal feedback mechanisms. Understanding of these functional properties pose major challenges on theoretical modeling approaches due to the complexities originating from spatio-temporal couplings over many length and time scales. Therefore an orchestrated modeling strategy is established on various scales, cf. the figure below, starting from molecular dynamics and Langevin simulations of nano- and meso-interfaces up to the reaction-diffusion treatment of the full nanoreactor continuum. After presenting tentative results and challenges on the latter, I will close by giving an outlook on how to embed my research within the ongoing activities in the Freiburg area.

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