Coarse-grained modelling of nanoparticle-polymer interactions

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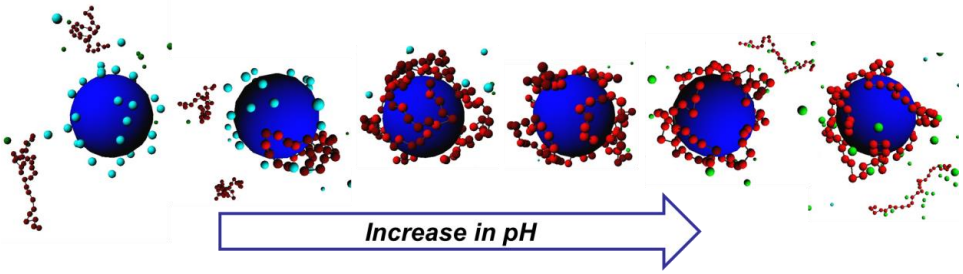
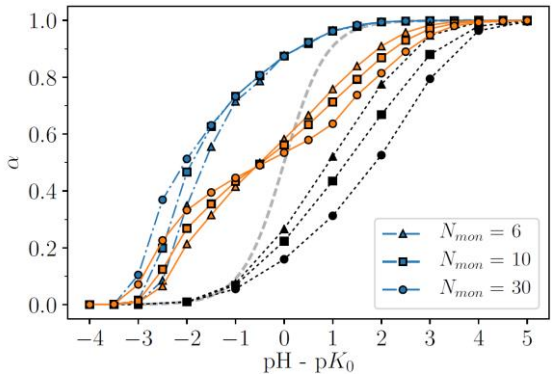
Systems comprising of nanoparticles (NPs) and oppositely charged polyelectrolytes are common components in formulations used in food, pharmaceutical and cosmetic formulations. In such applications, the presence of polymer chains that bridge two or more NPs can induce the aggregation of the NPs and consequent destabilization of the formulations.

In many applications as well as in biological systems, polymers are charged, which increases their solubility of the molecules in aqueous solution and prevents their aggregation.

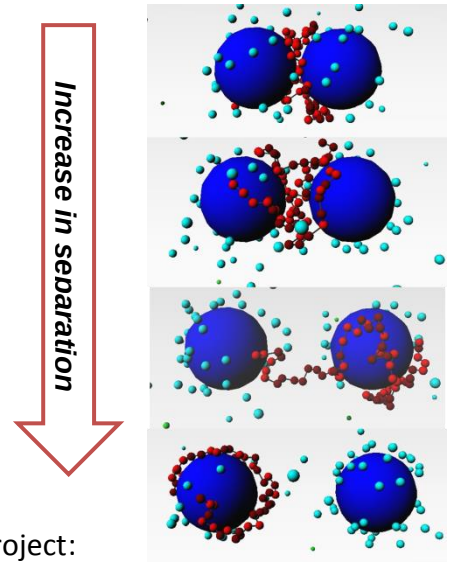
Within the class of charged polymers, weak polyelectrolytes present very interesting properties. Their charge can be tuned by variations in pH resulting in systems that can, in principle, respond to such external stimulus.

In this work we study systematically the effect of charge mobility (quenched vs. annealed) on the adsorption of polyacids (Pas) to NPs. The effect of PA chain length and number is evaluated, as well as the number of NPs.





Effect of PA chain length: titration curves of weak PA in the absence (black) and presence of a NP (R=1, blue and R=2, orange curves).



Students that have worked or are currently working in this project:
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