In silico investigation of magnetic water cleaning particles

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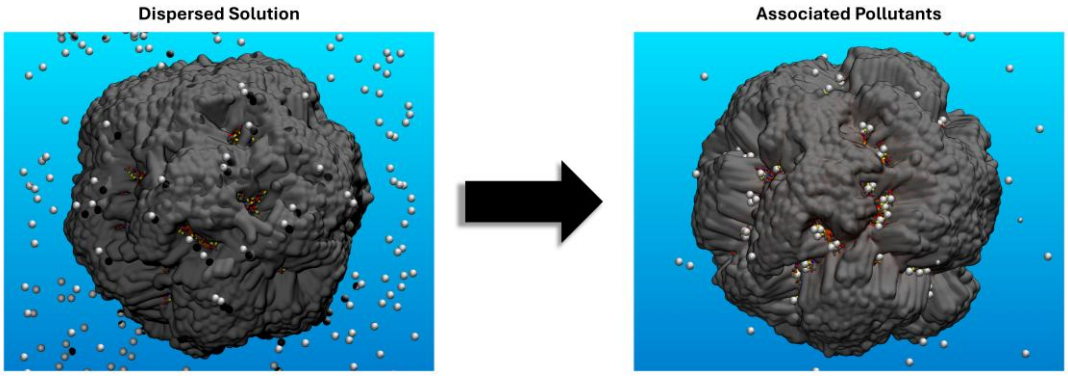
Clean water is among the most important resources and there is a continuously rising need for energy-efficient, simple upcycling methods. We use molecular modelling to tailor nanoparticle functionalization for cost-efficient recovery of polluted water. So far, this has been demonstrated for extracting crude oil [1], micro-/nanoplastics [2], glyphosate [3] and polychlorinated biphyenyls [4]. The carrier material is given by iron oxide nanoparticles that offer simple extraction via magnetic interactions. To enable molecular recognition of specific pollutant species, self-assembled monolayers (SAMs) consisting of phosphonic acid derivatives are bound to the nanoparticle surface. An exemplary system of a mixed SAM consisting of alkyl- and dimercapto functionalized phosphonic acids is depicted below, displaying its attractive character towards Hg^{2+} ions in aqueous solution.



We outline the assessment of unbiased molecular simulation models to describe the carriers, their functionalization by pure and mixed SAMs as functions of grafting density and the analyses of SAM-water interfaces. Based on such molecular understanding, dedicated molecular recognition motifs are envisaged to further boost pollutant extraction - whilst diminishing unwanted processes such as particle agglomeration.

REFERENCES

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