Polymer design for metal chelation
(in collaboration with Prof. Michael Schulz)

Polymers are promising candidates for metal ion extraction from complex solutions. Modelling can assist the design of such polymers by providing a fundamental understanding of the polymer-ion interaction at multiple time and length scales.

We develop parameters for the polarizable AMOEBA force field to accurately account for electrostatic effects. With classical molecular dynamics simulations, we can compute a binding affinity that includes both enthalpic and entropic contributions.

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Water in cortical bone

Bone’s unique properties stem from the hierarchical organization of a mineral (hydroxyapatite) and an organic (collagen) phase across multiple length scales. A key player in the integration of the organic and inorganic components of bone is water.

We contribute to the molecular understanding of the organization of organic and inorganic materials in bone. We use DFT MD to model this system and investigate the effects of confinement, collagen conformation and ionic concentration.

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References