## Molecular dynamics simulations of the interaction of Chondroitin 4sulphate with calcium oxalate monohydrate surfaces

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Calcium oxalate can be found in nature in three degrees of hydration: calcium oxalate monohydrate (COM,  $CaC_2O_4 \cdot H_2O$ , Whewellite), dihydrate (Weddellite), and trihydrate (Coaxite). Although the minerals are considered extremely rare in the geological environment[1], alkali earth oxalates nevertheless play an important role in nature and chemistry. The calcium salts of oxalic acid are also found in many plants, whereas COM is also present in more than 70% of renal calculi as the supersaturation conditions of the urine in the kidney nephrons favour the precipitation of COM into stones. One of the possible centres for its formation are the hydroxyapatite aggregates known as Randall's plaques, where the nucleation process is mediated by macromolecules, which are usually present in the organic matrix of the kidney stones

Glycosaminoglycans (GAGs) are polysaccharide molecules that are abundant in mineralised tissues. A GAG molecule is an unbranched polymer chain of two different types of monosaccharide linked together in alternation[2]. Normal urine contains about 2% GAGs, comprising about 60% sulphate (ChS). The literature Chondroitin reports contradicting results about the role of urinary GAGs; Some polysaccharides like Heparan (HS) are reported as inhibitors of growth and aggregation, while others such as ChS promote crystal nucleation in inorganic, artificial urine. Both ChS, derived from stone formers and HS have been reported to encourage the nucleation of COM crystals in urine[3].

In this work we use computational methods to investigate the interfacial interactions between ChS and COM. We present molecular dynamics (MD) simulations of Chondroitin 4-sulphate disaccharide adsorbed onto a slab of COM in the presence of interfacial water. Adsorption structures have been calculated for the dominant (100) surface, as well as the (010) and (121) surfaces, which are also found in the experimental morphology in the presence of aditives[4]. We have simulated the adsorption of the disaccharide components independently to isolate the essential COM–saccharide interactions for each adsorbate.

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