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Simulation of vaterite-aspartic acid interaction: model development and results

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Vaterite is a metastable anhydrous polymorph of calcium carbonate that is often produced through biological activity.[1,2] Here, biomolecules are believed to be the key to promoting its growth, inhibiting its dissolution or more generally to stabilising it. Recently, it has been found that chiral acidic amino acids can modify the organisation of vaterite crystallites depending on the enantiomer added during their formation and aggregation.[3] However, the atomic details of the formation of such specifically designed materials and of the specific role of the biomolecules are fully unexplored.

This presentation will focus on modelling the interaction between vaterite and the enantiomers of aspartic acid in water through classical molecular dynamics. The complexity of this apparently simple interaction and the challenges of developing a realistic, thermodynamically and kinetically predictive model will be discussed. The main results regarding the surface morphology of vaterite[4] and the interaction of aspartic acid with dissolved ions and vaterite will be presented.[5]

References:[1] Jacob *et al.; Nat. Commun.* 2017, 8, 1265.[2] Wightman *et al.*; *Flora* 2018, 241, 27.[3] Jiang *et al.; Nat. Commun.* 2017, 8, 15066.[4] Schuitemaker *et al. J. Chem. Phys.* 2021, 154, 164504.[5] Jiang *et al.; Nat. Commun.* 2019, 10, 2318.