Solvation and thermodynamic effects on small organic molecules on calcite

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Understanding how organic molecules interact with mineral surfaces is of major interest in a number of fields, including biomineralisation and enhanced oil recovery, and can offer significant environmental impacts and economic benefits. Molecular modelling techniques, such as density functional theory (DFT), provide a powerful means to complement experimental studies and gain insight into fundamental interaction between organic molecules and mineral surfaces. However, DFT calculations are generally performed in vacuum at 0 K, which can limit their applicability to investigations performed, for example, in solution at ambient temperature.

Our aim was to incorporate thermodynamics and solvation effects into the description of small organic molecule adsorption on mineral surfaces, specifically calcite. The thermodynamic results were obtained from explicit DFT calculations while the solvation effects were obtained using the COSMO-RS implicit solvent method. A model oil was also developed, which allows us to investigate the effect of multi-component solvent on the adsorption of the small organic molecules on calcite. This combined approach provided information about the adsorption behaviour of these small organic molecules on calcite in different realistic conditions, including a variety of temperatures and solution composition. The results indicate that solvation and thermodynamics affect the adsorption of the molecules on calcite significantly, with the latter dominating over the effect of solvation. Only a few of the small molecules are still stable on calcite in solution at 25 °C. Most of these molecules were less stable in the water phase than in the oil phase.