Atom-level modelling the free energy of Adsorption of Hazardous Compounds at soil-water Interfaces.

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The accumulation and persistence of hazardous compounds (HCs) in the environment has emerged as an adverse effect of human behaviour. HCs emerge from a variety of sources, including contaminants in personal care products, pesticides and manufacturing wastes. Some of these compounds have been shown to cause adverse effects in aquatic organisms, as well as increase the risk of developing thyroid disorders, tumours and diabetes in humans [1]

In this study, we aim to build on the foundations of our understanding of how HCs interact with the environment. We use atomistic simulation methods to determine the physicochemical factors controlling the distribution of pollutants and their metabolites in aqueous and terrestrial environments. This enables us to identify sustainable ways of control the transport of HCs and remediate their effect.

Our initial studies focused on the adsorption of HCs on model surfaces found in soil, such as the clays, sodium montmorillonite and pyrophyllite, ubiquitous silica and a model organic surface. We used a combination of dispersion corrected DFT and classical MD methods to calculate the binding free energy and identify favourable sites for HC adsorption on these organic and inorganic surfaces in vacuum and water. We then moved towards calculating the free energy of adsorption of these HCs at the mineral-water interfaces. The calculations proved too difficult using conventional simulation methods; hence we applied a new Monte-Carlo-based approach which allows the calculation to be efficiently parallelized [2]. By calculating the free energies of adsorption, we obtain insights into the behaviour of HCs at the soil-water interface and help to identify and potentially remediate highly persistent HCs.

[1] Petrie, B. et al.(2014) *Water Res*., **72**, 3–27

[2] Brukhno, A.V., (2019) *Mol Sim*, **45**, 1-21