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Exploring iron precipitation for understanding phosphate removal from wastewater

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Phosphorus is a vital nutrient for agriculture and fertiliser production. However, it is in limited supply across Europe, resulting in heavy dependence on imports. Promising substitutes for phosphorus recovery have been found to be municipal sewage sludge and wastewater [1]. But present techniques of removal mostly chemical precipitation with iron salts cause non-bioavailable iron phosphate species [2]. The molecular mechanisms of the initial steps of phosphate fixation with iron salts remain unclear due to the complex nature of the process and the many possible nucleating species involved. It is evident that iron hydroxides ($Fe(OH)_x$) play a crucial role in the mechanisms of phosphorus adsorption and precipitation [3]. Focussing on the early intermediates in iron hydroxide [4] precipitation and their reactivity towards phosphorus, this work seeks to clarify the molecular mechanisms underlying phosphorus fixation with iron salts during wastewater treatment. We examine the pH-dependent formation of iron hydroxide species and their subsequent conversion into iron phosphate compounds using 57Fe Mössbauer spectroscopy and density functional theory (DFT) calculations. DFT calculations have been performed with Gaussian 16 [5] to optimize the geometries of the structures shown in Fig.1 using the B3LYP functional and the CEP-31G basis set. Mössbauer parameters for these structures have been calculated using ORCA 6.0. [6], by applying the B3LYP functional along with the CP(ppp) basis set to analyse the electronic properties of iron atoms. The calculation of partial density of states is ongoing, and latest results will be presented.

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