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Evaluation of siderophores as compounds for the selective recovery of Indium and Germanium by means of density functional theory

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Siderophores are a diverse group of small of iron-chelating compounds which are secreted by a plethora of bacteria and fungi. In nature, their purpose is the sequestration of iron. However, due to their chemical characteristrics they are able to bind various other metals as well, making them promising compounds for the utilization in future green recycling technologies.

This work aims to find siderophores, that selectively complex the critical elements indium and germanium. As there are more than 500 different siderophores reported to this day, exhaustive experimental evaluation is highly impractical, though. Therefore, density functional theory (DFT) was utilized to model the complexation reactions and as a result estimate the affinities of the respective siderophores towards the metals of interest. With this in silico approach, siderophores that exhibited favourable binding energies were found and evaluated experimentally in order to verify the results obtained by theoretical means.

Proofing the suitability of siderophores for the selective recovery of indium and germanium from low-concentrated sources would pose as a first step in the creation of future applications of the compounds in a variety of bio-based recycling technologies, as they could aid to secure the supply of a multitude of strategic metals.