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Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: a molecular simulation study

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Abstract: In chemical and pharmaceutical industries, sulfur-containing compounds may exist in gas and liquid mixtures, and need to be removed. In this study, we report a molecular simulation study to investigate the adsorption and separation of *t*-butyl-mercaptan (TBM) in natural gas, as well as dimethyl sulfoxide (DMSO) in aqueous solution, by UiO-66 and its functional derivatives UiO-66-F_4, -$(CH_3)_2$, -$(COOH)_2$, -$(CF_3)_2$, and -naphthyl. It is revealed that the functional groups can act as additional adsorption sites and create stronger surface potential overlap, thus generally enhance adsorption capability. All the six UiO-66s show high adsorption capacity for TBM, except UiO-66-naphthyl due to reduced porosity and surface area. The TBM/CH_4 selectivity is predicted to be high in these UiO-66s, ranging from 2.2×10^4 to 2.4×10^5; intriguingly, the TBM separation is not affected by the presence of trace H_2O. The UiO-66s also exhibit good adsorption capacity and high selectivity for DMSO from aqueous solution, with DMSO/water selectivity up to 570 in UiO-66. This study provides microscopic insights into the selective adsorption of sulfur-containing compounds in both gas and liquid mixtures, and suggests that UiO-66s might be promising nanoporous materials for industry-relevant separation.

Keywords: UiO-66, sulfur, adsorption, separation, molecular simulation

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