H$_2$S Force Field Development and Adsorption in Fe-MOF-74

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H$_2$S is a very hazardous chemical and is of paramount concern to industries dealing with it as regards the health, safety and environment. The objective of our work is to find an optimum adsorbent for separating H$_2$S from the tail gas of the Claus Process. As a first step towards attaining this objective, the transferable potentials for phase equilibria (TraPPE) force field is extended to H$_2$S. The new model uses four interaction sites placed on the locations of the atoms together with a site located on the H-S-H bisector. The initial parameter screen focused on reproducing the experimental vapor–liquid coexistence curve of H$_2$S and its liquid-phase dielectric constant. The model is being further refined by considering the binary vapor–liquid equilibria of the H$_2$S – CH$_4$ and H$_2$S – CO$_2$ mixtures. The TraPPE model was used to compute the adsorption isotherm of H$_2$S in Fe-MOF-74, with Fe-MOF-74 described by the TraPPE-EH model with LoProP charges for the organic linkers and optimized parameters for the iron centers. In addition, optimized structures are obtained for the TraPPE H$_2$S model in various M-MOF-74 structures described by generic force fields and compared to electronic structure calculations.