

Accepted Manuscript

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

Wan Wei, Kang Zhang, Zhiwei Qiao, Jianwen Jiang

PII: S1385-8947(18)31496-7
DOI: <https://doi.org/10.1016/j.cej.2018.08.029>
Reference: CEJ 19643

To appear in: *Chemical Engineering Journal*

Received Date: 22 May 2018
Revised Date: 20 July 2018
Accepted Date: 5 August 2018

Please cite this article as: W. Wei, K. Zhang, Z. Qiao, J. Jiang, Functional UiO-66 for the removal of sulfur-containing compounds in gas and liquid mixtures: a molecular simulation study, *Chemical Engineering Journal* (2018), doi: <https://doi.org/10.1016/j.cej.2018.08.029>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



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

Wan Wei, Kang Zhang, Zhiwei Qiao and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576 Singapore

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-F₄, -(CH₃)₂, -(COOH)₂, -(CF₃)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/CH₄ 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 H₂O. 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

*E-mail: chejj@nus.edu.sg

Download English Version:

<https://daneshyari.com/en/article/10145331>

Download Persian Version:

<https://daneshyari.com/article/10145331>

[Daneshyari.com](https://daneshyari.com)