Structure–property Relationship for Separation of α-olefin/paraffin on Microporous Adsorbents: A Case for CuBTC Material

Ruihan Yang[1], Shafqat Ullah[2], Xiao Chen[1], Junxiang Ma[3], Yuan Gao[3], Yujun Wang[2], and Guangsheng Luo[2]

[1]Affiliation not available
[2]Tsinghua University
[3]Lu'an Chemical Group CO., LTD.

July 15, 2022

Abstract

Fishcher–Tropsch synthesis products contain ultrahigh-content α-olefins, which are of great value if the challenging separation of α-olefin/paraffin is achieved through energy-saving ways. Adsorption separation provides a promising alternative to distillation. One of the most significant differences between the adsorption separation of long-chain and light hydrocarbons is the steric hindrance of the molecular chain. Herein, a combination of window size, metal node spacing, and bending degree is proposed to quantitatively describe the structure–property relationship for the separation of long-chain α-olefin/paraffin on microporous materials. The adsorption capacity, selectivity, adsorption sites, and host–guest interactions of α-olefin/paraffin on CuBTC are investigated in detail to illustrate the structure–property relationship. The contributions of different interactions to the overall adsorption energy are innovatively quantified. This work guides the design of adsorbent structures and provides a generic approach to investigate the host–guest interactions during the adsorption or catalytic process of nanoporous materials.

Hosted file

`Manuscript.docx` available at https://authorea.com/users/495301/articles/577088-structure-property-relationship-for-separation-of-%CE%B1-olefin-paraffin-on-microporous-adsorbents-a-case-for-cubtc-material