Density Functional Theory Study of Tert-butylmercaptan (TBM) and Tetrahydrothiophene (THT) Adsorption on Modified ETS-10 and Activated Carbons

송호성, 한정우*
서울시립대학교
(jwhan@uos.ac.kr*)

Hydrogen is a non-toxic feedstock for chemical industry, and is an alternative fuel that may replace fossil fuel. Hydrogen production for residential fuel cells is an effective technology because numerous natural gas pipelines are almost reaching home in many areas. However, it is required to separate organosulfur compounds such as tert-butylmercaptan (TBM) and tetrahydrothiophene (THT) added in fuel gas for preventing from poisoning catalysts in fuel cells. Na,K-ETS-10, Cu-ETS-10, activated carbons (AC), and AC-HNO3 are considered as promising adsorbents for removal of organosulfur compounds. Here, we performed density functional theory calculations to obtain the information for designing the desulfurization method by investigating TBM and THT adsorption. We reveal how each absorbent affects the adsorption energies of TBM and THT, and suggest a way of how to increase their adsorption capacities.