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An atomistic approach of thiophene hydrodesulfurization over γ-Mo2N catalyst

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In this study, we investigate the gas phase Hydrodesulfurization (HDS) mechanism of thiophene over a molybdenum nitride γ-Mo_2N (111) surface by means of Density Functional Theory (DFT). Geometry optimizations suggest that thiophene preferentially adsorbs in a flat mode over a 3-fold fcc nitrogen hollow site with physisorbed energy of -48.8 kcal/mol. From thermodynamics and kinetic considerations, two reaction mechanisms, termed as Direct Desulfurization (DDS) and Hydrogenation (HYD) are investigated. Due to the sizable activation barrier required for the first C-S bond scission of 54.6 kcal/mol, we found that the proposed Direct Desulfurization pathway is highly unlikely to proceed. However, the addition of hydrogen atoms to the adsorbed thiophene reduces the energy barriers for the first C-S bond scission to be 24.1 kcal/mol followed by formation butadienyl adduct and an adsorbed sulfur atom (C_4H_6+S). Further hydrogenation of the unsaturated hydrocarbons (i.e., C_4H_6) results in the production of 2-Butene (i.e., partially hydrogenation) and butane (i.e., full hydrogenation). Reaction rate calculations infer that 2-hydrothiophene is the slowest reaction. Furthermore, estimated rate constants for the sulfur removal at temperature of 373 K and 573 K amount to 1.46×10^{4} s^{-1}.active $site^{-1}$ - 1.73×10^{10} s^{-1}.active $site^{-1}$; respectively. Results provided in this paper highlight promising industrial applications of crystalline molybdenum nitride catalysts toward high selectivity of partial hydrogenation of alkynes into alkenes and removal of sulfur content from cyclic hydrocarbons.

Biography

Zainab Naji Jaf has completed her Master's degree from College of Education for Pure Sciences - Ibn Al-Haitham Department of Physics, University of Bagdad, Iraq. She is currently pursuing her PhD degree.

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