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Computational modeling of Cu@furfural imine-decorated halloysites as the efficient catalyst in regioselective synthesis of triazoles

Tayebeh Hosseinnejad[1] and **Samahe Sadjadi**[2]
[1]Alzahra University, Iran
[2]Polymer and Petrochemical Institute, Iran

Halloysite nanotubes (HNTs), with general formula of ($Al_2(OH)4Si_2O_5.2H_2O$) possess high surface area, tubular morphology and high mechanical strength. In HNTs a monolayer of water separates the unite layers in HNTs. Moreover, the exterior and interior surfaces of HNTs are chemically different. Tetrahedral SiO_4 groups are located in the outer surface while the octahedral gibbsite $Al(OH)_3$ sheet forms the inner surface. Recently, functionalization of the surface of HNTs and immobilization of metal nano particles are considered as a potent method for modification of the features of HNTs and expanding their applications specially as an effective catalyst in the selective synthesis of an specific isomer of pharmacetual compounds. In continuation of our attempt to introduce computational modeling of structural, electronic and thermochemical properties of heterogeneous nanocatalysts to design the regioselective synthesis of 1,2,3-triazoles as pharmacetual compounds, herein, we present a novel heterogeneous catalyst based on functionalization of HNTs with (3-chloropropyl) trimethoxysilan, thiosemicarbazide and furfural and incorporation of copper NPs. Considering the importance of understanding the surface chemical and physicochemical properties of functionalized HNTs, we investigated the computational modeling of regioselective synthesis of disubstituted 1,2,3-triazoles. Strictly speaking, we concentrated on the quantitative description of structural and electronic features of interactions between copper NPs and thiosemicarbazide functionalized HNTs modified with furfural (denoted as HNTs-T-F) via density functional theory (DFT) and quantum theory of atoms in molecules (QTAIM) approaches. Then, we applied our computational modeling in the design of reaction path so that it can be led to the synthesis of an specific isomer of disubstituted 1,2,3-triazoles as pharmacetual compounds.

Biography

Tayebeh Hosseinnejad received his BSc, MSc and PhD degrees from University of Tehran in 2001, 2003 and 2007 respectively. She completed his Doctoral thesis under supervision of Prof. Hassan Behnejad. She joined as an Assistant Professor in Alzahra University, Iran. Her research interests focuses on computational organic and organometallic chemistry and computational thermodynamics.

tayebeh.hosseinnejad@alzahra.ac.ir

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