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Modeling HDS reactions. Interaction of benzothiophene with the 'WNiS', 'WPdS', and 'WPtS' type catalysts. A DFT Study.

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Catalytic hydroprocessing is a relevant process in petroleum refining industry for impurities removal of hydrocarbon, ranking from straight-run naphta to vacuum residue or even heavy and extra heavy oils. When handling heavy feeds, hydroprocesing has the ability to increase the yield of destillates and simultaneously reduce the contents of sulfur, nitrogen, metals (Ni, V) and asphaltenes. We use the DFT (ADF) methodology, contained in the package of molecular modeling Cerius2, to study the study the benzothiophene adsorption on the model bimetallic clusters $W_2H_2NiS_8$, $W_2H_2PdS_8$ and $W_2H_2PtS_8$. We found many interesting results: 1. The pi adsorption of the benzothiophene (BT), on the model catalytic surfaces, it is preferred ; 2. The energy and the shape of the frontier orbitals, HOMO and LUMO for the adsorbate and the catalytic surface, respectively, give us the better view of the interactions in these systems.

The results obtained in this work suggest the following conclusions: i. There is an optimal atomic relation (M/M+W) , M = Ni, Pd, Pt, for which the interaction with BT is favored ; ii. The pi adsorption mode of the BT molecule on the catalytic surfaces is privileged ; iii. The LUMO orbital of the catalytic surfaces and HOMO of the BT permit us tu predict the better interactions.

Key words: HDS, DFT, Heavy oil, metallic promoters

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