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Theoretical study of the adsorption of alcohols on H-ZSM-5 zeolite

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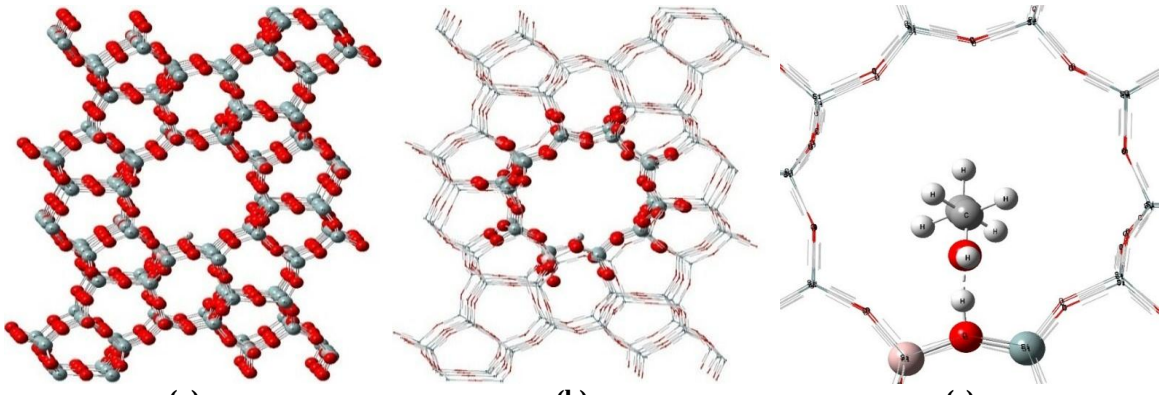
Demand for energy and raw materials derived from non-renewable sources of energy such as coal, oil and natural gas has increased rapidly in recent years and has been fueling the search for alternatives to renewable sources [1]. Plastic, gasoline, rubber, paints and other materials can be produced from the catalytic alcohols dehydration on surfaces of adsorbents formed by oxides or aluminosilicates [1,2,3]. The main objective of this work is the theoretical study of the adsorption of methanol, ethanol, propanol and n-butanol in a specific pore of zeolite H-ZSM-5 (Figure 1 a-c). The calculations were performed with the Gaussian09 package using classical, semi-empirical and DFT methods in combinations with two different layers of theory through the ONIOM hybrid method.

Key-words: Adsorption, H-ZSM-5, alcohols, ONIOM



(a) **(b)** **(c)**

Figure 1. (a) H-ZSM-5 zeolite model, (b) specific pore e (c) Complex model of H-ZSM-5/alcohol.

The adsorbent and adsorbate models were optimized separately and together (cluster) for energy analysis. The results showed bond energy variation with the relaxation of the central pore tetrahedron of H-ZSM-5. The effect was more accentuated with the heavier alcohols for both the hybrid methods: ONIOM2-PM6/UFF and ONIOM2-DFT/UFF, as shown in Figure 2 (a) e (b), indicating that the the adsorption with the zeolite is dependent on the size of the alcohols.

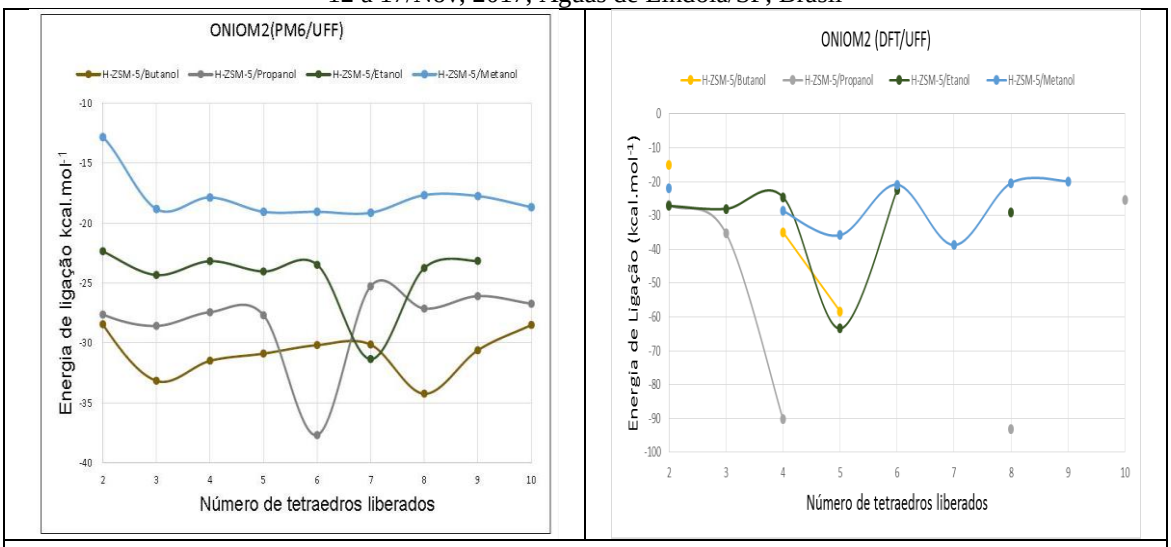


Figure 2. Bonding energy vs tetrahedron number obtained with (a) ONIOM2-PM6/UFF and (b) ONIOM2-DFT/UFF.

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