A DFT STUDY ON ZIRCONIA OLIGOMERS AND THE INFLUENCE OF CU-DOPING.

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A theoretical study of Zirconia-based linear oligomers $(ZrO_2)_n$ (n=1-5) has been performed in order to compare its intrinsic reactivity with the number of ZrO_2 units and the adsorption of Cu atoms. DFT-based indexes such as chemical potential (μ), hardness (η), Fukui (FF) and the dual Fukui (DF) functions were used with the aim of characterize the intrinsic reactivity on the studied clusters. B3LYP/6-31G** calculations with Lanl2dz pseudopotentials on metallic centers indicate that the ability to charge transfer and reactivity increases with the number of ZrO_2 units.

The Fukui function and the dual Fukui descriptor indicates that the nucleophilic character resides at the oxygen atoms and the electrophilic character is centered at Zr atoms. $Cu(ZrO_2)$ and $Cu(ZrO_2)_2$ clusters were analyzed and compared to (ZrO_2) and $(ZrO_2)_2$, it is found that while the nucleophilic character resides at Cu atoms being larger than at copper-free clusters, the electrophilic character remains centered at the Zr atoms.

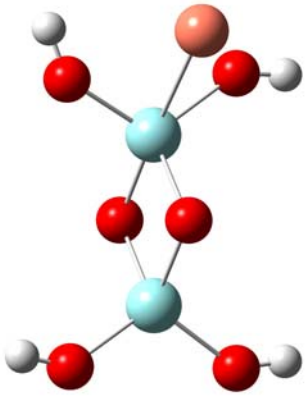

Figure1: $Cu(ZrO_2)_2$ Cluster.

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