Density functional theory investigation of NO$_2$ and SO$_2$ adsorption on isolated and anatase-supported BaO clusters$^1$ MUSTAFA TEK, HANDE USTUNEL, Department of Physics, Middle East Tech University, Ankara, Turkey, DANIELE TOFFOLI, Department of Chemistry, Middle East Tech University, Ankara, Turkey — BaO is the most commonly used storage component in NO$_x$ storage and reduction catalysts (NSR). TiO$_2$ has recently been suggested by several authors as a promising support material, with increased sulphur tolerance when compared with traditional supports such as $\gamma$-Al$_2$O$_3$. The optimization of NSR catalysts requires knowledge of the interaction between the storage and support components. In this talk, we present a DFT investigation of the electronic and structural properties of NO$_2$ and SO$_2$ adsorption on isolated and anatase-supported (BaO)$_n$ ($n=1,2,4,6,8,9$) clusters. Generally, supported BaO clusters are found to display better tolerance towards sulphur poisoning compared to both bare BaO (100) surface and supported BaO overlayers.

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