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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 γ-Al_2O_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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