DFT Study of Adsorption of H2, N2 and CO2 on the Surface of Hematite Nanocatalysts for Green Urea Synthesis

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Abstract. α-Fe2O3 (hematite) nanoparticles were synthesized using sol-gel method. The hematite was calcined using tube furnace at 600°C temperature and ambient pressure. XRD analysis was conducted to confirm the formation of the desired nanoparticles. The magnetic properties of the nanoparticles was studied using Vibrating Sample Magnetometer (VSM). The single-phase formation and high crystallinity of hematite was confirmed using XRD. The saturation magnetization of hematite is 6.901 emu/g. The coercivity of hematite has the value of 3841.3 G. The adsorption energy of sorbates gases on the surface of sorbents nanocatalysts with different clave surfaces were calculated using Adsorption Locators module. Band structure and density of states of reactant gas molecules with nanocatalysts were calculated using Cambridge Seriel Total Energy Package (CASTEP) module.