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# Scavenging performance and antioxidant activity of γ-alumina nanoparticles towards DPPH free radical: Spectroscopic and DFT-D studies

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## ABSTRACT

The radical scavenging performance and antioxidant activity of γ-alumina nanoparticles towards 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical were investigated by spectroscopic and computational methods. The radical scavenging ability of γ-alumina nanoparticles in the media with different polarity (i.e. *i*-propanol and *n*-hexane) was evaluated by measuring the DPPH absorbance in UV-Vis absorption spectra. The structure and morphology of γ-alumina nanoparticles before and after adsorption of DPPH were studied using XRD, FT-IR and UV-Vis spectroscopic techniques. The adsorption of DPPH free radical on the clean and hydrated γ-alumina (1 1 0) surface was examined by dispersion corrected density functional theory (DFT-D) and natural bond orbital (NBO) calculations. Also, time-dependent density functional theory (TD-DFT) was used to predict the absorption spectra. The adsorption was occurred through the interaction of radical nitrogen $N^{\bullet}$ and $NO_2$ groups of DPPH with the acidic and basic sites of γ-alumina surface. The high potential for the adsorption of DPPH radical on γ-alumina nanoparticles was investigated. Interaction of DPPH with Brønsted and Lewis acidic sites of γ-alumina was more favored than Brønsted basic sites. The following order for the adsorption of DPPH over the different active sites of γ-alumina was predicted: Brønsted base < Lewis acid < Brønsted acid. These results are of great significance for the environmental application of γ-alumina nanoparticles in order to remove free radicals.

**Keywords:** γ-Alumina, DPPH, Antioxidant, Radical scavenger, Adsorption, DFT

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