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Synthesis, characterization and application of  $\text{Fe}_3\text{O}_4@\text{SiO}_2$  nanoparticles supported palladium(II) complex as a magnetically catalyst for the reduction of 2,4-dinitrophenylhydrazine, 4-nitrophenol and chromium(VI): A combined theoretical (DFT) and experimental study

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# Synthesis, characterization and application of $\text{Fe}_3\text{O}_4@\text{SiO}_2$ nanoparticles supported palladium(II) complex as a magnetically catalyst for the reduction of 2,4-dinitrophenylhydrazine, 4-nitrophenol and chromium(VI): A combined theoretical (DFT) and experimental study

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## ABSTRACT

In the present work, a new catalytic system based on palladium(II)-tetrazole complex immobilized on silica-coated  $\text{Fe}_3\text{O}_4$  ( $\text{Fe}_3\text{O}_4@\text{SiO}_2$ ) nanoparticles ( $[\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-Tet-Pd(II)}]$ ) is introduced. In the first stage, the geometry optimization and calculations of structural and electronic properties of molecular system 5-phenyl-1*H*-tetrazole-Pd (II) complex have been carried out at UB3LYP/6-31G\*/LANL2DZ level of theory. Then, the  $[\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-Tet-Pd(II)}]$  was prepared via immobilizing 5-phenyl-1*H*-tetrazole as a suitable ligand on the surface of  $\text{Fe}_3\text{O}_4@\text{SiO}_2$  as a support. The  $[\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-Tet-Pd(II)}]$  as a novel magnetically catalyst was characterized by XRD, FT-IR, FE-SEM, EDS, TG-DTA and VSM. This heterogeneous catalytic system demonstrated high activity in the reduction of 2,4-dinitrophenylhydrazine (2,4-DNPH), 4-nitrophenol (4-NP) and Cr(VI) in the present of  $\text{NaBH}_4$  as the reduction agent at room temperature and was reusable five times with no obvious decrease of catalytic activity.

**Keywords:** Palladium complex; Theoretical studies;  $[\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-Tet-Pd(II)}]$ ; Magnetic nanocatalyst; Reduction; Cr(VI); Nitro compounds

## 1. Introduction

Recently, metal complexes have attracted much attention in different areas such as biotechnology, materials science and modern chemistry [1]. In general, the metal complex has a central metal atom or ion and one or more ligands.

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