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Palladium acetate supported on amidoxime-functionalized magnetic cellulose: synthesis, DFT study and application in Suzuki reaction

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Highlights

- The magnetic cellulose composite was well-designed and synthesized.
- A quantitative description of metal–ligand interactions was assessed.
- High catalytic activity obtained for Suzuki cross-coupling reaction.
- The magnetic composite takes on favorable reusability.

Abstract

A highly efficient and magnetically retrievable catalytic system involving Pd (II) acetate supported on amidoxime-functionalized cellulose nano-magnetic catalyst (nano-Fe₃O₄@AOFC/Pd(II)) was prepared. The structure of the organic-inorganic hybrid nanocomposite has been confirmed using various physicochemical techniques such as FT-IR, XRD, TGA, VSM, XPS, HRTEM, SAED, SEM, CHNS, EDAS and ICP-OES. In addition, to describe and go insight to the metal–ligand interactions present in the nano-Fe₃O₄@AOFC/Pd (II) composite, covalent and electrostatic interactions, density functional theory (DFT) model and quantum theory of atoms in molecule method were employed. The resultant nano-magnetic cellulose composite exhibits remarkable catalytic efficacy used for Suzuki cross-coupling reaction

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