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In situ preparation and characterization of novel CuI-functionalized poly[(methyl methacrylate)-co-maleimide] as an efficient heterogeneous catalyst in the regioselective synthesis of 1,2,3-triazoles via click reaction: Experimental and computational chemistry

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Abstract

A CuI-functionalized poly[(methyl methacrylate)-co-maleimide] (CuI@[PMMA-co-MI]) nanocatalyst was prepared from in situ polymerization and functionalization of poly[(methyl methacrylate)-co-(maleic anhydride)] and well characterized using various techniques. From a computational viewpoint, we assessed two complexation models between copper nanoparticles and [PMMA-co-MI]. In this line, the metal–ligand interaction strength was also studied via density functional theory calculations and frontier molecular orbital analysis. Moreover, for presenting a quantitative description of the electronic features of immobilization of copper nanoparticles on polymeric support, the topological analysis of electron density and its Laplacian was performed through quantum theory of atoms in molecules. Finally, the catalytic activity of CuI@[PMMA-co-MI] as a heterogeneous nanocatalyst was successfully

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examined in the highly regioselective synthesis of 1,4-disubstituted 1,2,3-triazoles via click reaction.

Keywords: click reaction, CuI@[PMMA-co-MI] nanocatalyst, density functional theory, organometallic catalyst, polymer-supported catalyst