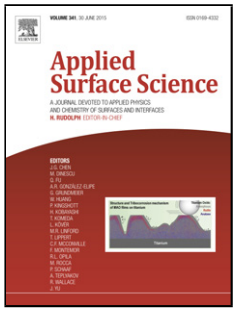

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Heterogeneous hydrogenation using stable and reusable calix[4]pyrrole fenced Pt nanoparticles and its mechanistic insight

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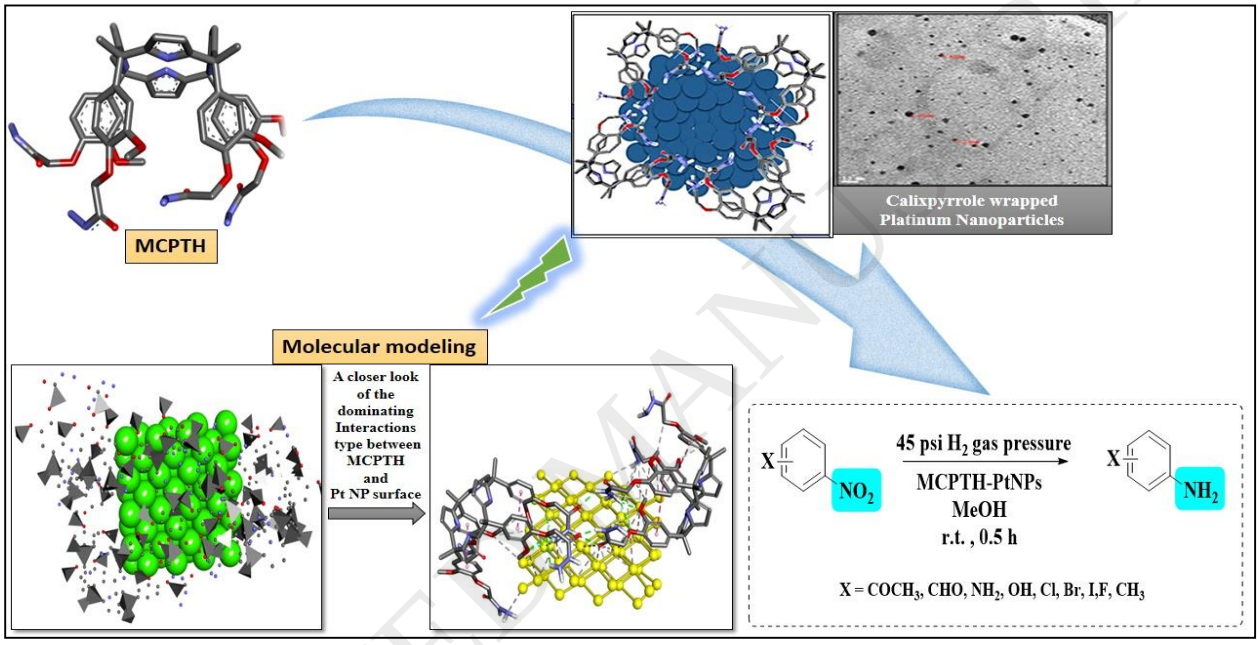
Graphical Abstract



Abstract:

Novel calix[4]pyrrole encapsulated platinum nanoparticles (PtNPs) have been prepared in aqueous medium using meso-tetra(methoxy) meso-tetra (4-phenoxy acetohydrazide) calix[4]pyrrole (MCPTH) as both reducing as well as capping agent. MCPTH-PtNPs nano-assembly has been characterized by HRTEM, XRD, XPS, TGA and FTIR methods. Subsequently, we envisaged the grafting of the MCPTH on the PtNPs by molecular dynamics simulations that renders towards the complemented role of MCPTH in capping the surface *via* metal-acceptor interactions. These nanoparticles have been exploited for chemoselective hydrogenation of nitroarenes using molecular hydrogen at room temperature. Supplemented computational and experimental apprehension clearly corroborates that hydrazide group remains in close contact with the surface and provides adequate coordination sites for the adsorption of nitrenes; required for hydrogenation. This catalytic approach can be conceive as an important tool for determining the electronic and structural influence on the catalytic activity which may open new vistas pertaining to the use of calix functionalized nanocatalyst.

Keywords: Calix[4]pyrrole; Platinum nanoparticles; Molecular modelling; Catalysis; Nitroarene reduction