Supplementary to:

Mesoporous Silica Beads Encapsulated with Functionalized Palladium Nanocrystallites: Novel Catalyst for selective Hydrogen generation

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Graph5.TIF

***Figure S1****. XPS survey spectrum of different nanocomposites used for the analysis.*

xrd bead.tif

***Figure S2****. XRD spectra for Pd/GO/EETMS*

**Investigation on porosity of silica alginate beads :**

silica exp.tif

***Figure S3****. Pictorial representation of the effect of concentration of alkoxysilanes on the porosity of silica beads. Figures 1-5 (anticlockwise), elucidates with time leaching of nanomaterial from the silica beads in case of lower content of alkoxysilanes (0.5 M) (b), in comparison to (a) where significant amount of alkoxysilane (2.5 M) is present.*

The presence of alkoxysilanes in the synthetic route of Palladium nanocrystallites effectively controls the pore size of calcium alginate beads to the order of 2-10 nm, thereby creating a mesoporous matrix for nanomaterial encapsulation. Figure S1 shows the effect of concentrations of alkoxysilanes on maintaining the mesoporous character of the silica alginate beads entrapped with Palladium nanocomposites. Figure 2S shows the enlarged view of mesoporous (pore size 2-10 nm) silica alginate beads with lower and higher alkoxysilane content, and its significant effect on the pore size of the beads.

pore.tif

***Figure S4****. Optical micrographs showing the enlarged view of the silica beads, depicting the variation in pore sizes with the concentration of silica, 1) 0.5 M and 2) 2.5 M. Inset to figure 2 represents the mesoporous silica beads*

The proposed mechanism for the evolution of hydrogen is as follows:

where catalyst is **Pd/GO/EETMS - 623K.**

reaction.tif

***Figure S5****. Mechanism of hydrazine decomposition based on the FTIR investigations.*

**Table SI. Summary of values of d-spacing corresponding to the lattice planes obtained in synthesized Palladium nanocomposites.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Nanocomposites | d-spacing  [111] | d-spacing  [200] | d-spacing  [220] | d-spacing  [222] | d-spacing  [311] | d-spacing  [400] | d-spacing  [422] |
| Pd/GPTMS | 2.124 | - | - | 1.118 | - | 0.966 | 0.832 |
| Pd/ EETMS | 2.144 | 1.747 | 1.320 | - | 1.173 | - | - |
| Pd/GO/EETMS | 2.231 | 1.956 | - | - | - | - | - |
| Pd/GO/GPTMS | 2.102 | - | - | - | 1.170 | - | - |