## Supporting Information:

# Screening of Heterogeneous Multimetallic Nanoparticle Catalysts Supported on Metal Oxides for Mono-, Poly-, and Heteroaromatic Hydrogenation

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**Table S1**. Quantities of Reagents Required for Desired Support Composition.

| **Support Composition** | **EtOH (ml)** | **1.788 M $Al(OBu)_3$ (ml)** | **Titanium (IV) isopropoxide (ml)** | **TEOS (ml)** | **$EtOH/HCl/H_2O$ (ml)** |
|---|---|---|---|---|---|
| $Al_2O_3$ | 11.3 | 11.2 | 0 | 0 | 8.1 |
| $SiO_2$ | 5.6 | 0 | 0 | 2.18 | 4.1 |
| $TiO_2$ | 5.6 | 0 | 3.0 | 0 | 4.1 |
| $Al_2O_3$(25%)- $SiO_2$(75%) | 7.0 | 2.8 | 0 | 1.64 | 5.1 |
| $Al_2O_3$(50%)- $SiO_2$(50%) | 8.4 | 5.6 | 0 | 1.09 | 6.1 |
| $Al_2O_3$(75%)- $SiO_2$(25%) | 9.8 | 8.4 | 0 | 0.545 | 7.1 |
| $Al_2O_3$(25%)- $TiO_2$(75%) | 7.0 | 2.8 | 2.25 | 0 | 5.1 |
| $Al_2O_3$(50%)- $TiO_2$(50%) | 8.4 | 5.6 | 1.5 | 0 | 6.1 |
| $Al_2O_3$(75%)- $TiO_2$(25%) | 9.8 | 8.4 | 0.75 | 0 | 7.1 |
| $SiO_2$(25%)- $TiO_2$(75%) | 5.6 | 0 | 2.25 | 0.545 | 4.1 |
| $SiO_2$(50%)- $TiO_2$(50%) | 5.6 | 0 | 1.5 | 1.09 | 4.1 |
| $SiO_2$(75%)- $TiO_2$(25%) | 5.6 | 0 | 0.75 | 1.635 | 4.1 |


**Figure S1.** Screening plate containing 96 vials.

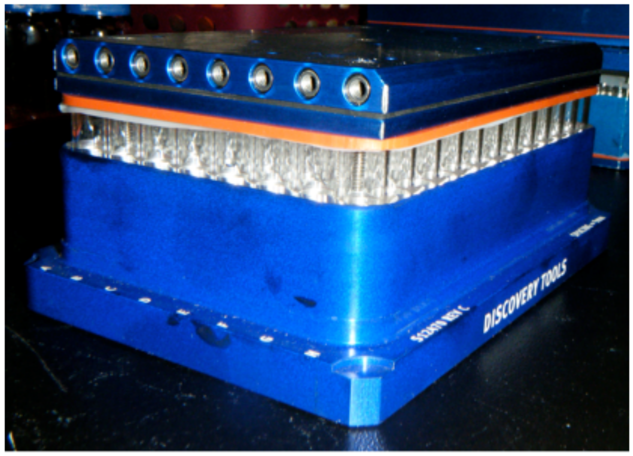


**Figure S2.** Assembled screening plate with top plate.

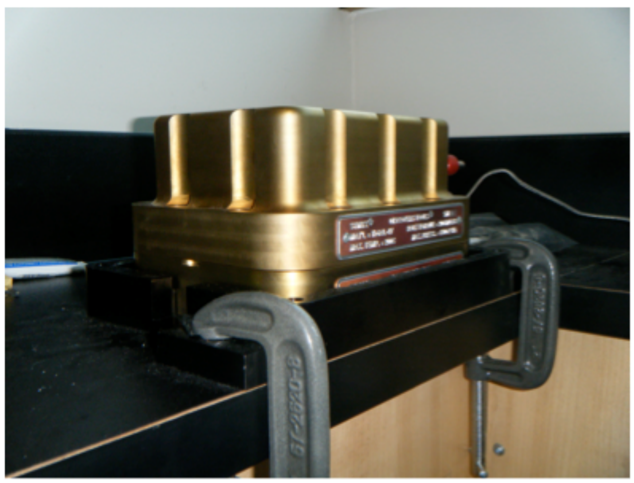

**Figure S3.** Batch reactor.

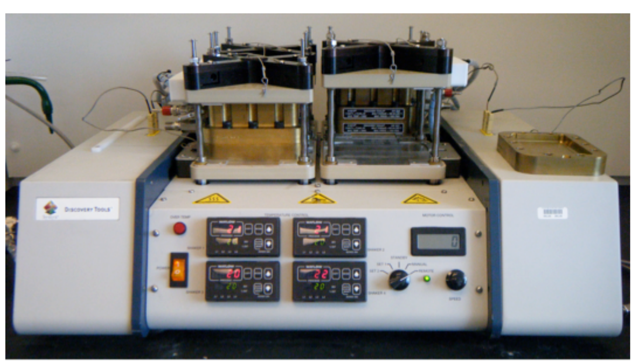

**Figure S4.** Heated orbital shaker system (HOSS).

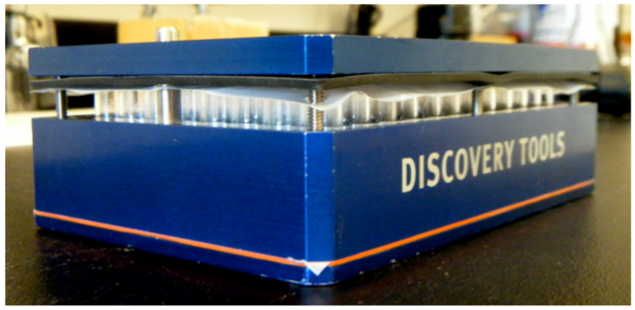


**Figure S5.** Plate used for GC-MS analysis.

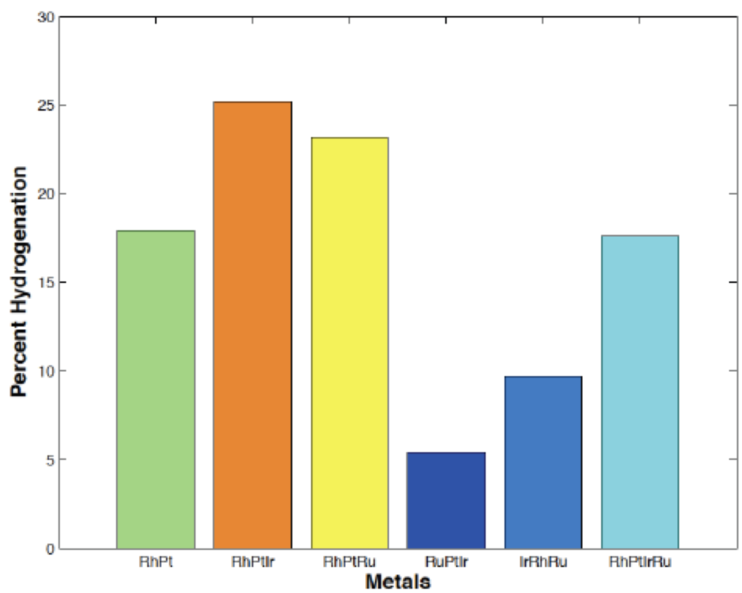


**Figure S6.** Tri- and tetra-metallic toluene hydrogenation results. All of the catalysts were supported on $Al_2O_3$ and had a total metal loading of 1%. The percent hydrogenation of toluene was measured after 4 hours and was determined by gas chromatography.

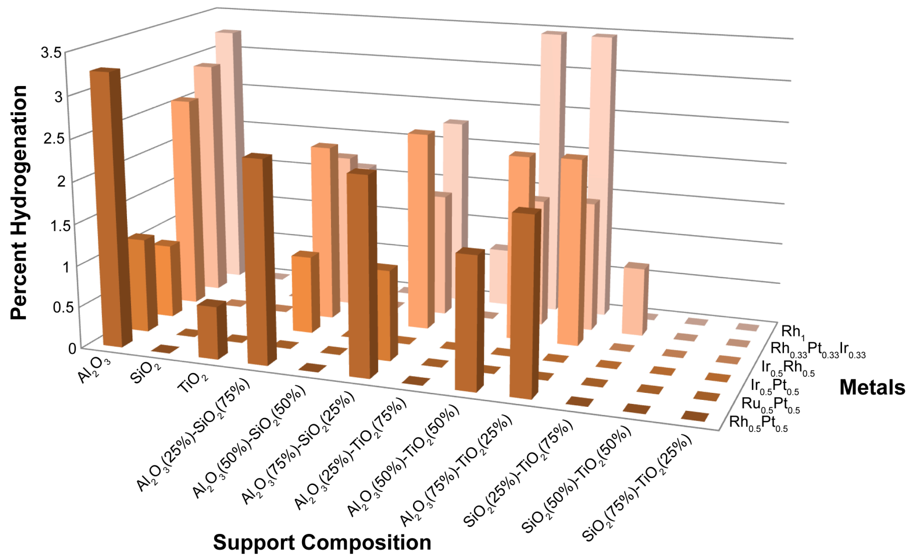


**Figure S7.** Benzothiophene screening results.

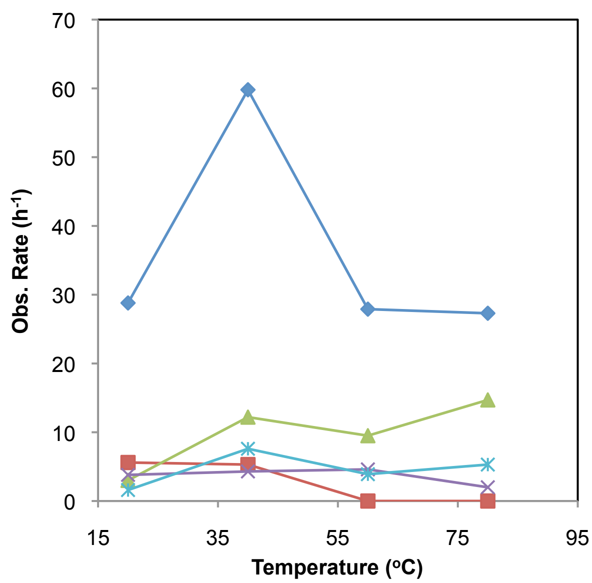


**Figure S8.** Observed initial rates for the hydrogenation of naphthalene at 20 atm $H_2$ and various temperatures using select catalysts. Blue: commercial 0.5% $Rh/Al_2O_3$ catalyst. Red: $Rh_1/Al_2O_3$(25%)-$SiO_2$(75%) catalyst. Green: $Rh_1/Al_2O_3$ catalyst. Purple: $Rh_{0.5}Pt_{0.5}/Al_2O_3$ catalyst. Turquoise: $Rh_{0.33}Pt_{0.33}Ir_{0.33}/Al_2O_3$ catalyst.

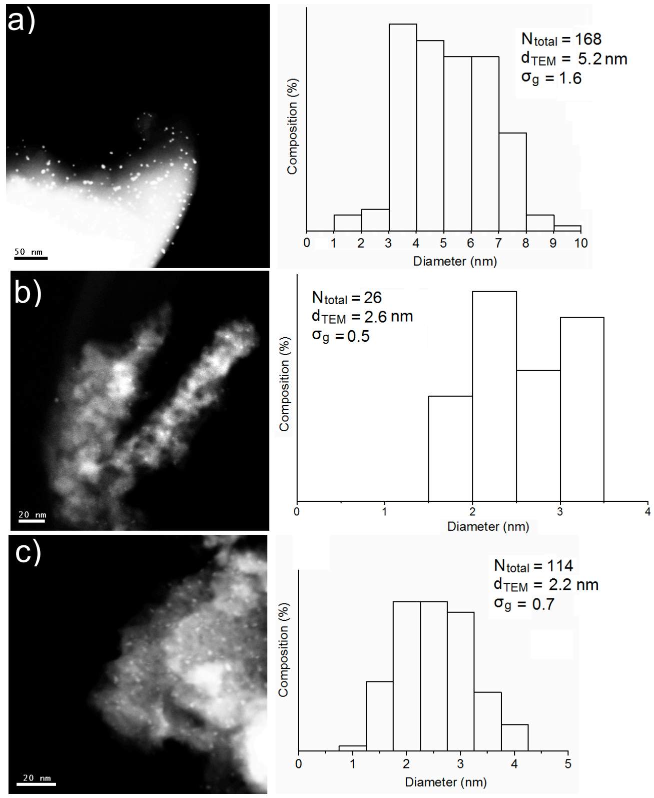


**Figure S9.** Pre-catalysis TEM images and NP size histograms of a) $Rh_1/SiO_2$, b) $Rh_1/Al_2O_3$, and c) $Rh_1/TiO_2$.

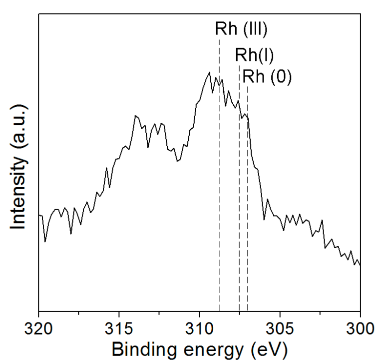


**Figure S10.** Pre-catalysis high resolution XPS spectra of Rh in $Rh_1/Al_2O_3$(25%)-$SiO_2$(75%). The Rh 3d peak binding energy is 308.7 eV, which suggests that the Rh is oxidized to Rh(III).

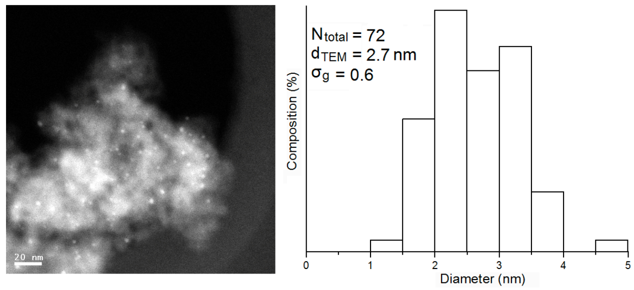


**Figure S11.** Pre-catalysis TEM images and particle size histograms for $Rh_{0.33}Pt_{0.33}Ir_{0.33}/Al_2O_3$.

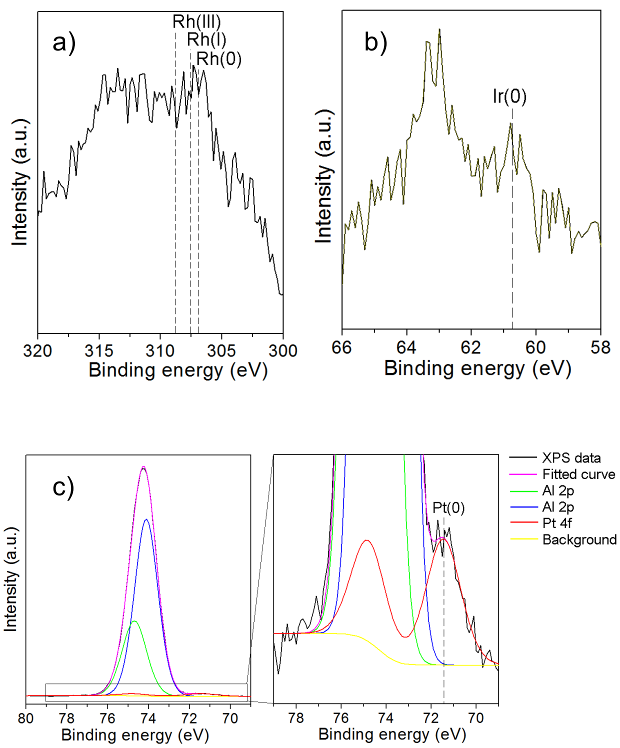


**Figure S12.** Pre-catalysis high resolution XPS spectra of a) Rh, b) Ir and c) Pt in $Rh_{0.33}Pt_{0.33}Ir_{0.33}/Al_2O_3$. The Rh 3d peak has a binding energy of 306.9 eV indicating that it is in the zero oxidation state. The apparent Ir $4f_{7/2}$ peak is at 60.7 eV, which corresponds to Ir(0). The Pt 4f peak at 71.4 eV indicates that it is Pt(0).

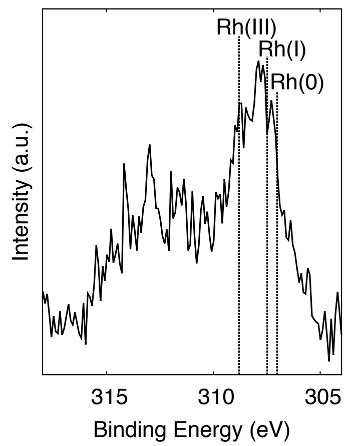


**Figure S13.** Pre-catalysis high resolution XPS spectra of Rh in $Rh_1/Al_2O_3$. The Rh 3d peak has a binding energy of 308.0 eV, suggesting that the Rh is slightly oxidized.

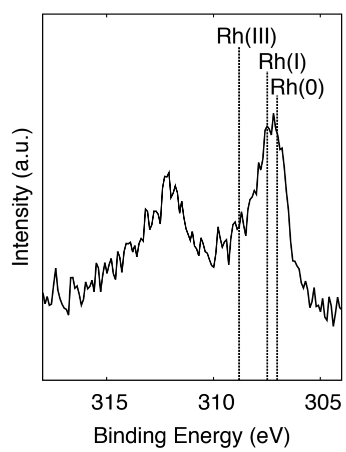


**Figure S14.** Pre-catalysis high resolution XPS spectra of Rh in $Rh_1/SiO_2$. The Rh 3d peak has a binding energy of 307.4 eV.

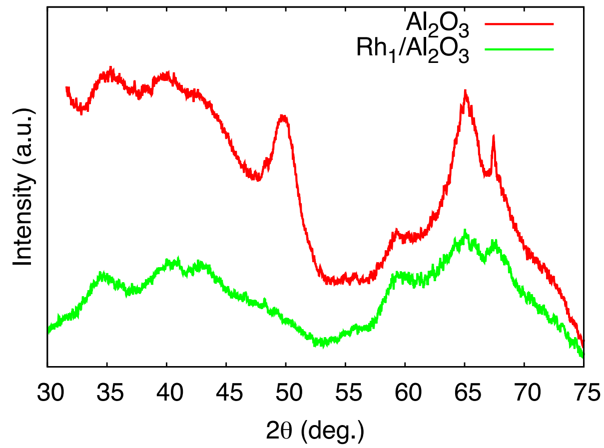


**Figure S15.** XRD patterns of $Al_2O_3$ and $Rh_1/Al_2O_3$.

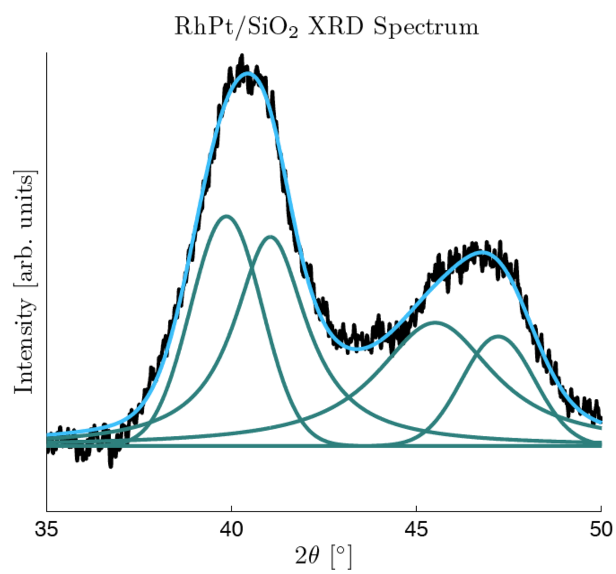


**Fig. S16.** Fitting procedure for $Rh_{0.5}Pt_{0.5}/SiO_2$ sample. In order to determine the integral breadth and peak centre, the XRD profile is fit to a series of Lorenztian peaks after background subtraction. The grain size is determined via the Scherrer equation: $D = \lambda / (\beta * \cos(\theta))$ where $\lambda$ is the wavelength of the probing radiation (1.54056 Angstrom), $\beta$ is the integral width of the fit peak and $\theta$ is centre position of the peak.