Metallosurfactant based Pd-Ni Alloy Nanoparticles as proficient catalyst in Mizoroki Heck Coupling Reaction

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Supplementary Information

S1: Spectroscopic data (^{1}H NMR) of entries 1-8 of Table 1

Entry 1, 2 and 6. (*E*)-Stilbene, A white solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 7.16 (s, 2H, *H*C=C*H*), 7.25 (d, 2H, Ar-H), 7.35 (t, 4H, Ar-H), 7.51 (d, 4H, Ar-H) ppm.

Entry 3. (*E*)-4-Methoxystilbene, A white solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 3.83 (s, 3H, OCH_3), 6.90 (d, 2H, Ar-H),), 6.98 (d, *J*H-H = 16.0 Hz, 1H, *H*C=CH), 7.07 (d, *J*H-H = 16.0 Hz, 1H, HC=C*H*), 7.23 (d, 1H, Ar-H), 7.35 (t, 2H, Ar-H), 7.45 (d, 2H, Ar-H), 7.49 (d, 2H, Ar-H) ppm.

Entry 4 and 7. (*E*)-4-Nitrostilbene, A yellow soli; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 7.14 (d, 1H, Ar-H), 7.26 (d, *J*H-H = 16.4 Hz, *H*C=CH), 7.33 (m, 2H, Ar-H), 7.40 (d, *J*H-H = 16.4 Hz, HC=C*H*), 7.55 (d, 2H, Ar-H), 7.63 (d, 2H, Ar-H), 8.22 (d, 2H, Ar-H) ppm.

Entry 5. (*E*)-4-Cyanostilbene, A white solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 7.09 (d, *J*H-H = 16.0 Hz, 1H, *H*C=CH), 7.21 (d, *J*H-H = 16.0 Hz, 1H, HC=C*H*), 7.32 (t, 1H, Ar-H), 7.39 (t, 2H, Ar-H), 7.53 (d, 2H, Ar-H), 7.58 (d, 2H, Ar-H), 7.63 (d, 2H, Ar-H) ppm.

Entry 8. (*E*)-4-Acetylstilbene, A yellow solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 2.61 (s, 3H, $COCH_3$), 7.13 (d, 1H, Ar-H), 7.23 (d, *J*H-H = 16.0 Hz, 1H, *H*C=CH), 7.30 (d, *J*H-H = 16.0 Hz, 1H, HC=C*H*), 7.38 (t, 2H, Ar-H), 7.54 (d, 2H, Ar-H), 7.59 (d, 2H, Ar-H), 7.95 (d, 2H, Ar-H) ppm.

Entry 9, 10, 14. (E)-Ethylcinnamate, yellow oily liquid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 1.35 (t, 3H, CH_3), 4.27 (q, 2H, CH_2), 6.44 (d, J *J*H-H =15.6 Hz, 1H, HC=C*H*), 7.40-7.37 (m, 3H, Ar-H), 7.54-7.51 (m, 2H, Ar-H), 7.69 (d, *J*H-H =16.0 Hz, 1H, *H*C=CH) ppm.

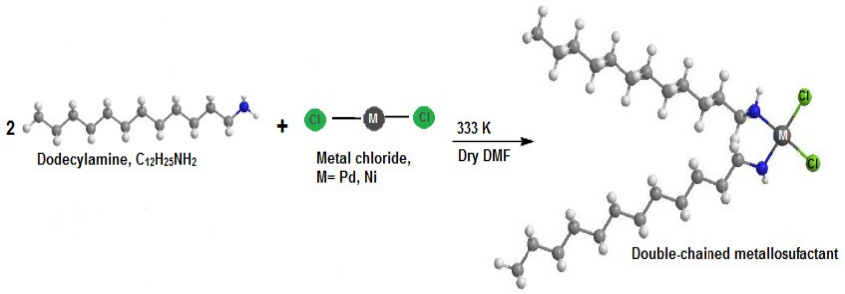
Entry 11. (E)-Ethyl 3-(4-methoxyphenyl)acrylate, colorless solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 1.32 (t, 3H, CH_3), 3.80 (s, 3H, OCH_3), 4.25 (q, 2H, CH_2), 6.46 (d, *J*H-H =15.8 Hz, 1H, HC=C*H*), 7.46-6.87 (m, 4H, Ar-H), 7.64 (d, *J*H-H =16 Hz, 1H, *H*C=CH) ppm.

Entry 12, 15. (E)-Ethyl 3-(4-nitroyphenyl)acrylate, yellow oily liquid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 1.35 (t, 3H, CH_3), 4.29 (q, 2H, CH_2), 6.68 (d, *J*H-H =16 Hz, 1H, HC=C*H*), 7.72-7.66 (m, 2H, Ar-H), 7.78 (d, *J*H-H =16 Hz, 1H, *H*C=CH), 8.25-8.24 (m, 2H, Ar-H) ppm.

Entry 13. (E)-Ethyl 3-(4-cyanophenyl)acrylate, yellow solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 1.35 (t, 3H, CH_3), 4.29 (q, 2H, CH_3), 6.54 (d, *J*H-H =16 Hz, 1H, HC=C*H*), 7.46-7.50 (m, 4H, Ar-H), 7.69 (d, *J*H-H =16 Hz, 1H, *H*C=CH) ppm.

Entry 16. (E)-Ethyl 3-(4-acetoxyphenyl)acrylate, solid; ^{1}H NMR (400MHz, $CDCl_3$, 25°C, TMS): δ = 1.34 (d, 3H, CH_3), 2.61 (s, 3H, CH_3), 4.27 (q, 2H, CH_2), 6.49 (d, *J*H-H = 16 Hz, 1H, HC=C*H*), 7.61-7.60 (m, 2H, Ar-H), 7.68 (d, *J*H-H = 16 Hz, 1H, *H*C=CH), 7.97-7.96 (m, 2H, Ar-H) ppm.

Scheme S1: Synthesis of complex 1 (M = Pd) and complex 2 (M = Ni)



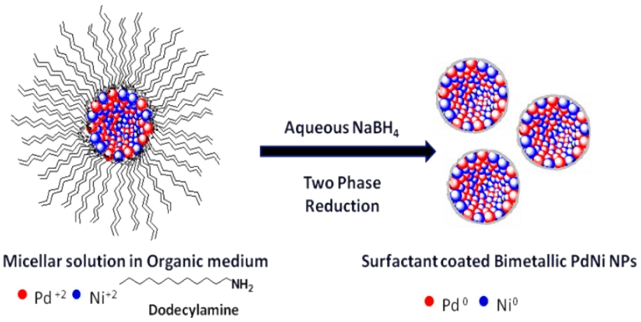


Fig. S1 Schematic representation of the synthesis of NPs.

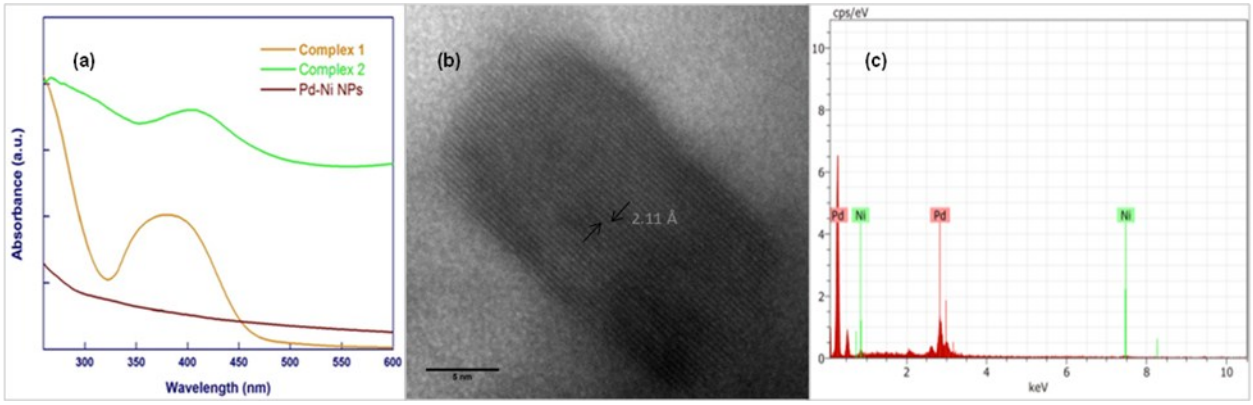


Fig. S2 (a) UV-Vis spectrum (b) HRTEM (c) EDS image of Pd-Ni Nps

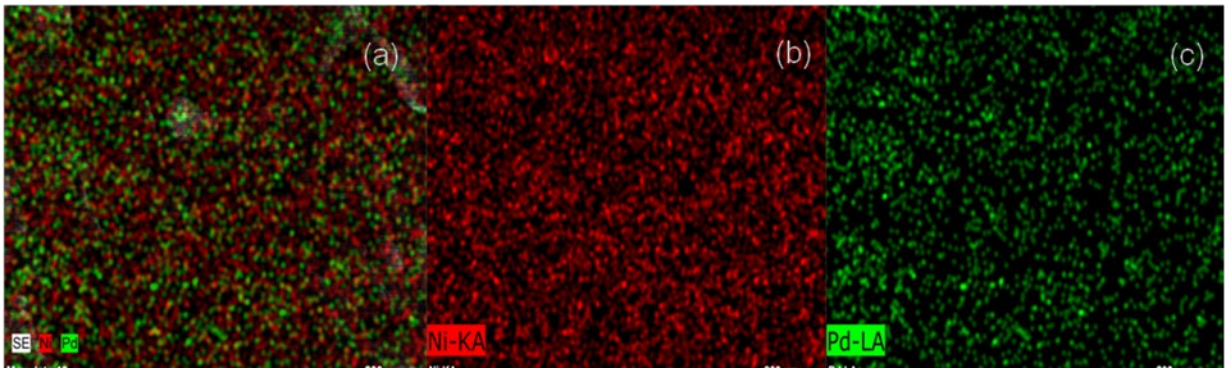


Fig. S3 Elemental maps of region of FESEM image highlighting (a) both Ni and Pd (b) Ni (c) Pd

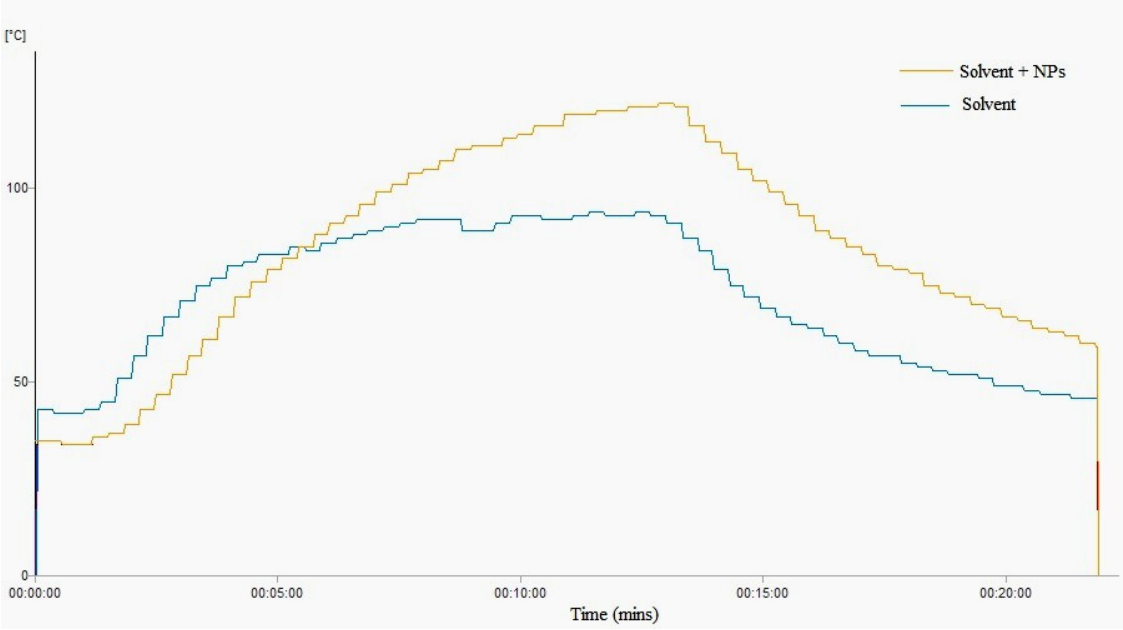


Fig. S4 Comparison of temperature profiles of system carrying blank solvent and solvent with NPs.

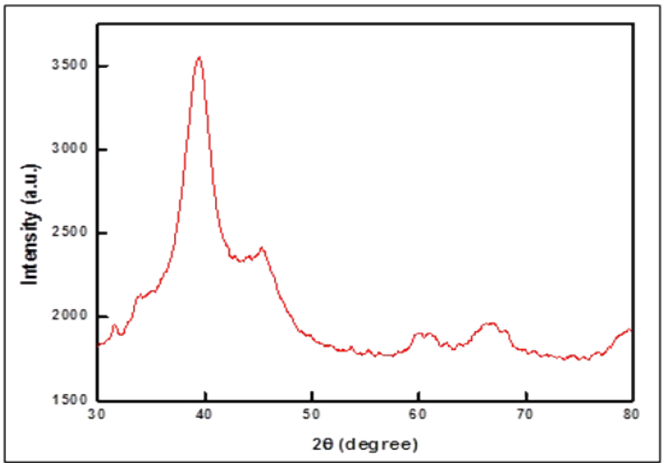


Fig. S5 XRD pattern of Pd-Ni NPs recovered after five catalytic cycles

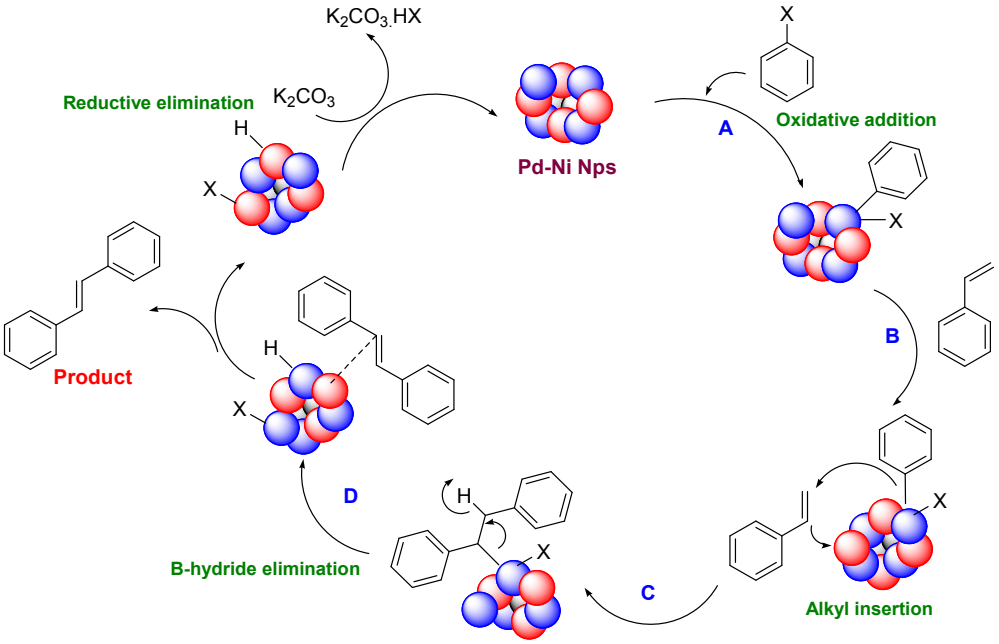


Fig. S6: Plausible mechanism of the reaction between styrene and halobenzene on NP surface.

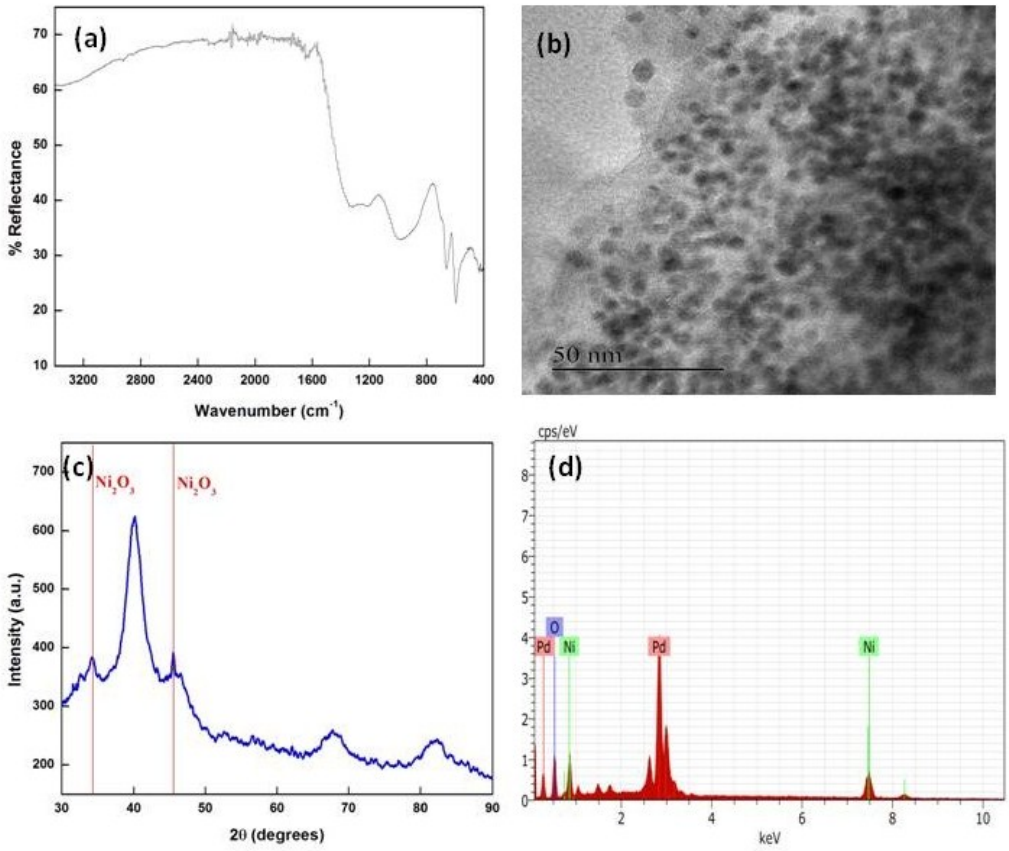


Fig. S7 (a) IR spectrum (b) TEM image (c) XRD pattern and (d) EDS of calcined Pd-Ni NPs.