Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Coating of Pd/C catalysts with Lewis-acidic ionic liquids and liquid coordination complexes – SCILL induced activity enhancement in arene hydrogenation

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Batch autoclave setup

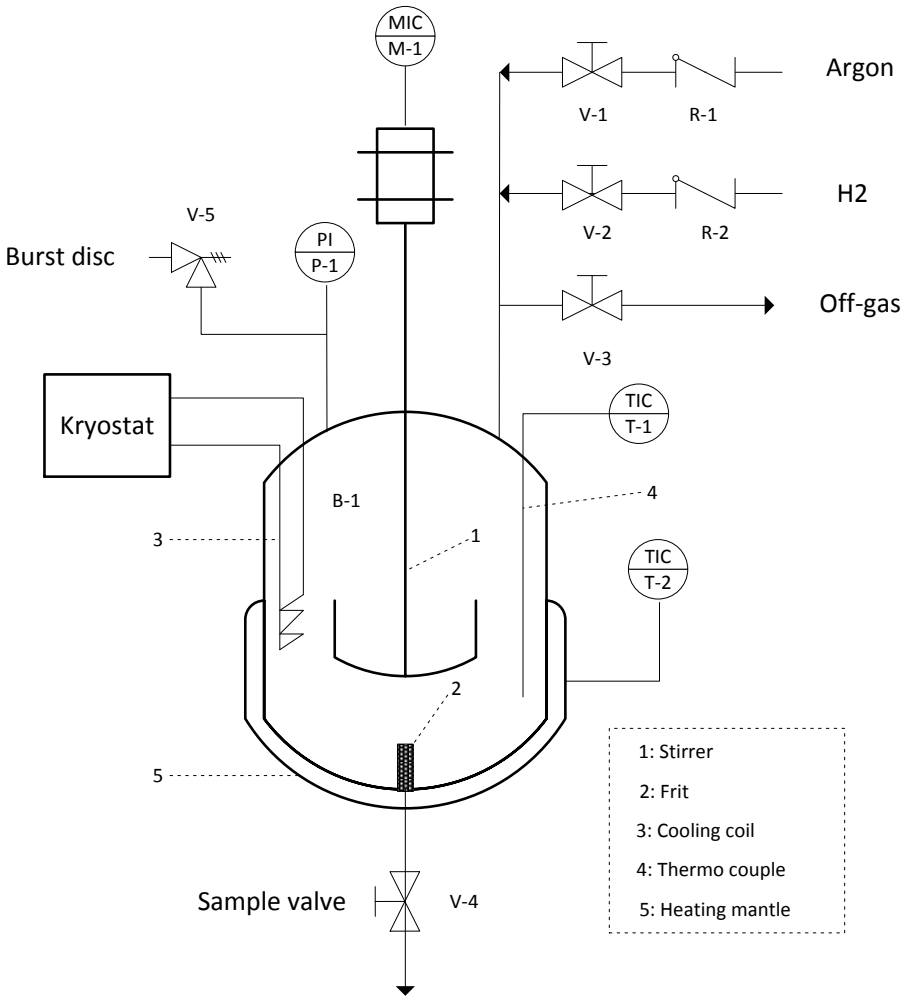

Figure S1. Schematic flow sheet (left) and photograph (right) of the batch reactor utilized.

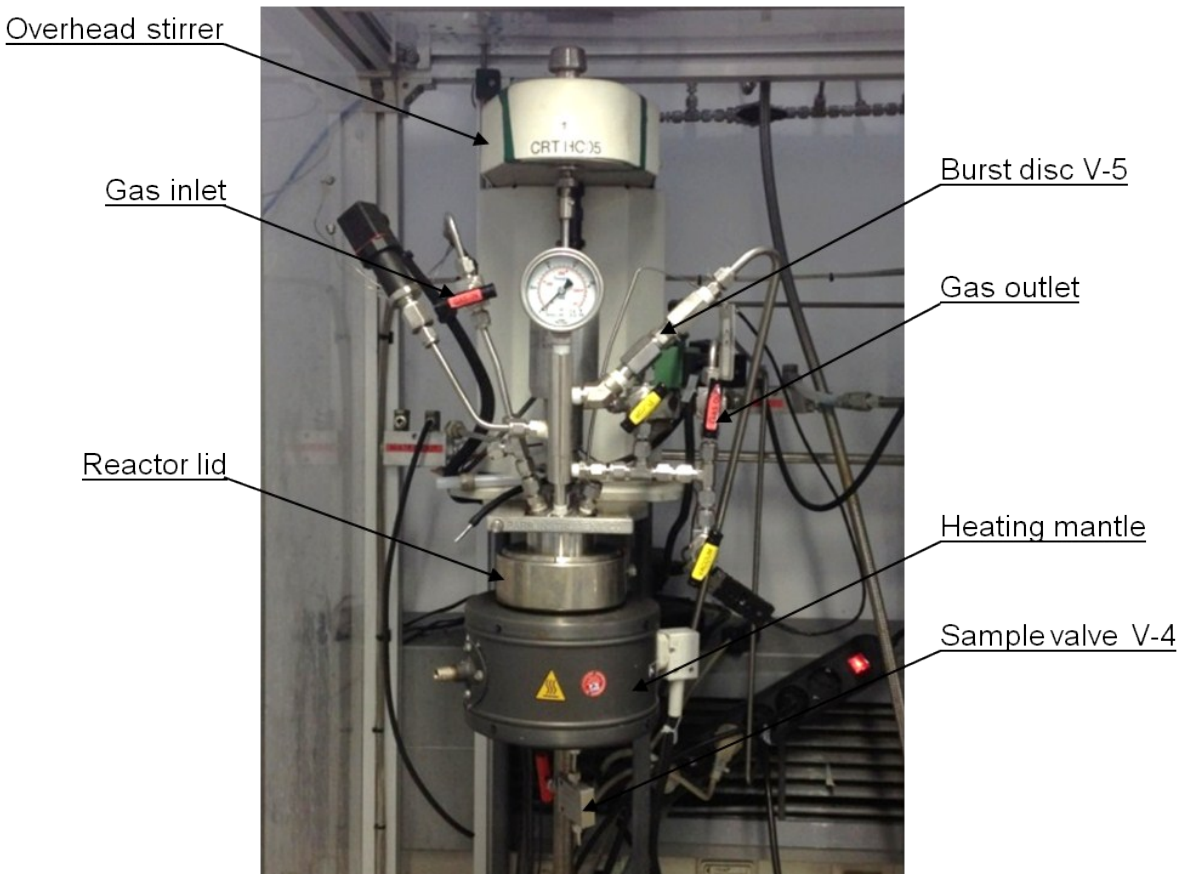

Figure S2. Photograph of the assembled reactor.

Comparison between addition of AlCl3 and [BMIM]Cl/$AlCl_3$ in bulk and SCILL

Figure S3 shows the conversion time plots for uncoated Pd/C without and with addition of [BMIM]Cl/$AlCl_3$ (x_{AlCl3} = 0.67). The amount of ionic liquid added was adjusted to the same amount of $AlCl_3$ present in a Pd-SCILL-**1** system, namely approx. 13 % or 41.3 mg.

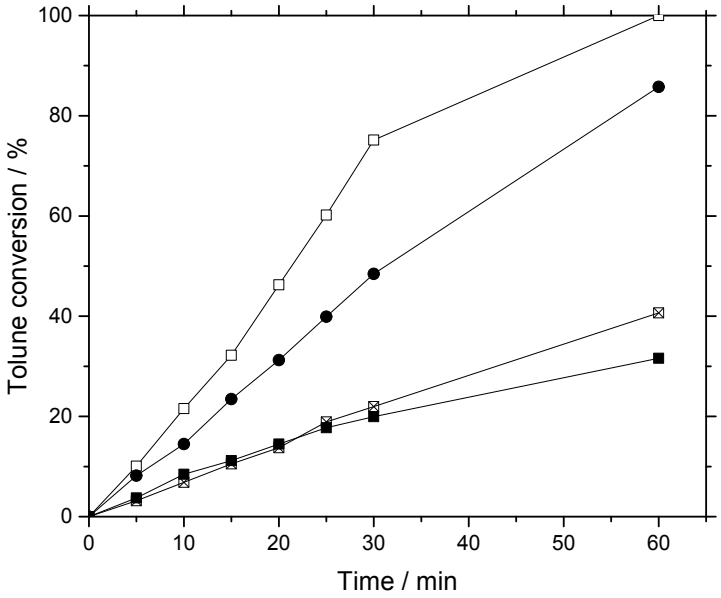

Figure S3. Conversion over time for toluene hydrogenation using Pd/C, with 330 mg (open squares), 41.3 mg (open squares intersected) and without (filled squares) addition of $AlCl_3$, as well as Lewis-acidic chloroaluminate Pd-SCILL-**1** catalysts (filled circles). Reaction conditions: T = 60 °C, $p_{hydrogen}$ = 15 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 1000 min^{-1}. Ionic liquid = [BMIM]Cl/$AlCl_3$ (x_{AlCl3} = 0.67).

Textural analysis of the Pd-SCILL-1 catalyst

The Pd-SCILL-**1** catalyst, coated with chloroaluminate ionic liquid, was analyzed by means of N_2 sorption at 77 K on a Quadrasorb-SI from Quantachrome. The data are compiled in Table S1.

Table S1. Textural data for the Pd-SCILL-**1** catalyst containing varying amounts of chloroaluminate ionic liquid [BMIM]Cl/$AlCl_3$ (x_{AlCl3} = 0.67).

Catalyst	Ionic liquid wt%	Surface area $m^2\ g^{-1}$	Pore volume mL g^{-1}	Av. Pore diameter nm
Pd/C	-	921	0.67	2.9
Pd-SCILL-**1**	6	393	0.47	4.8
Pd-SCILL-**1**	17	283	0.31	4.4
Pd-SCILL-**1**	45	146	0.18	4.8

Temperature variation in toluene hydrogenation

The uncoated Pd/C catalyst was tested in the temperature range between 40 and 80 °C.

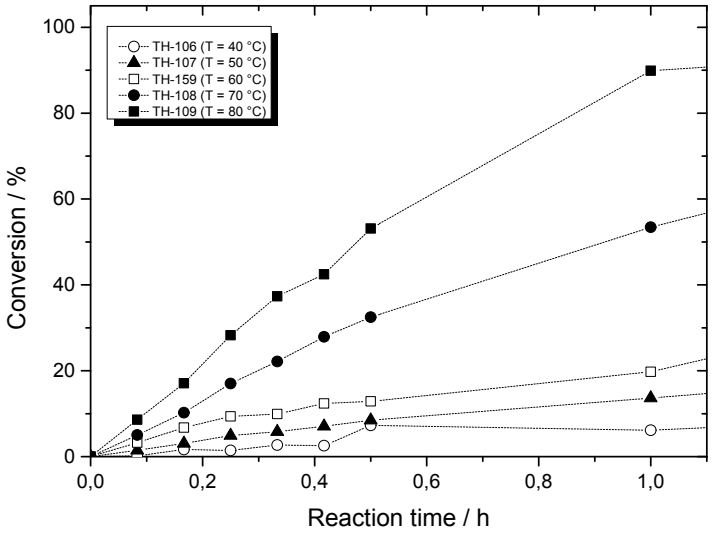

Figure S4. Conversion over time plot for the hydrogenation of toluene using Pd/C catalyst. Reaction conditions: $p_{hydrogen}$ = 15 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 1000 min^{-1}, ionic liquid coating = 13 wt%.

The chloroaluminate coated Pd-SCILL-**1** catalyst was tested in the temperature range between 40 and 80 °C.

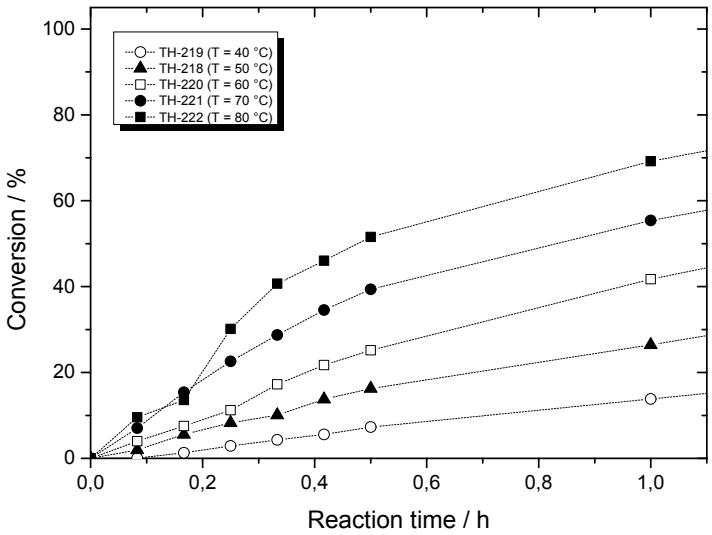

Figure S5. Conversion over time plot for the hydrogenation of toluene using Pd-SCILL-**1** catalyst. Reaction conditions: $p_{hydrogen}$ = 15 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 1000 min^{-1}, ionic liquid coating = 13 wt%.

The LCC coated Pd-SCILL-**2** catalyst was tested in the temperature range between 40 and 90 °C.

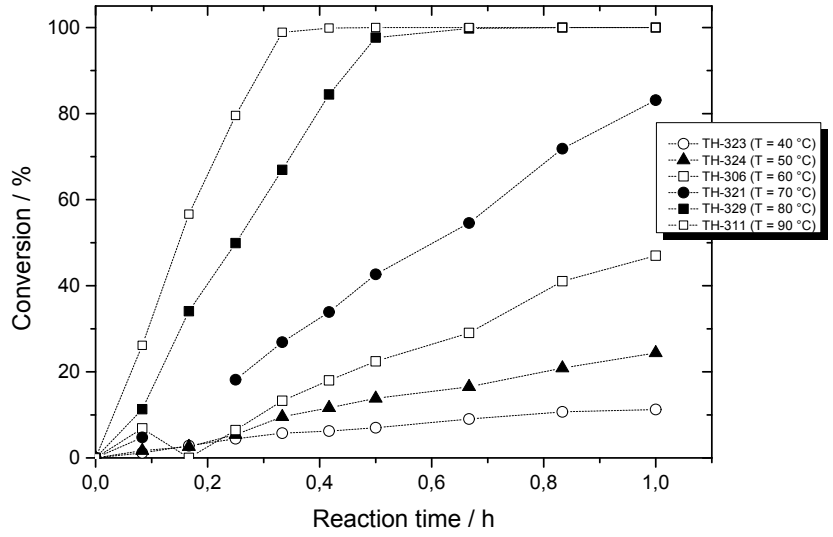

Figure S6. Conversion over time plot for the hydrogenation of toluene using Pd-SCILL-**2** catalyst. Reaction conditions: $p_{hydrogen}$ = 15 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 1000 min^{-1}, ionic liquid coating = 13 wt%.

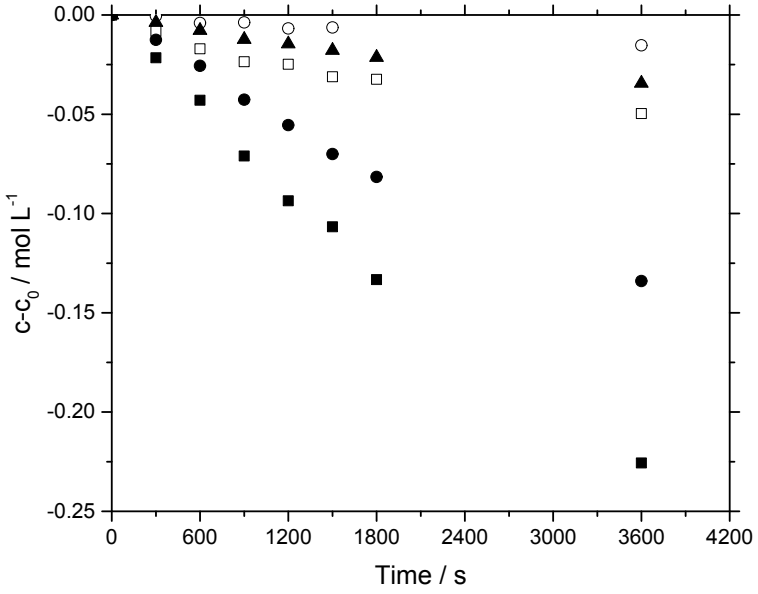

Figure S7. Integral analysis of toluene hydrogenation using Pd/C catalysts. Temperatures as indicated in Figure S3.

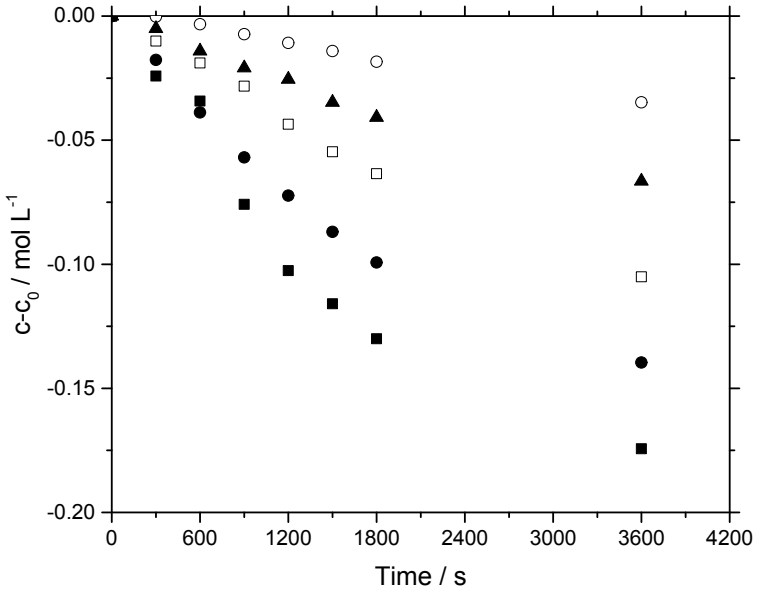

Figure S8. Integral analysis of toluene hydrogenation using Pd-SCILL-**1** catalysts. Temperatures as indicated in Figure S4.

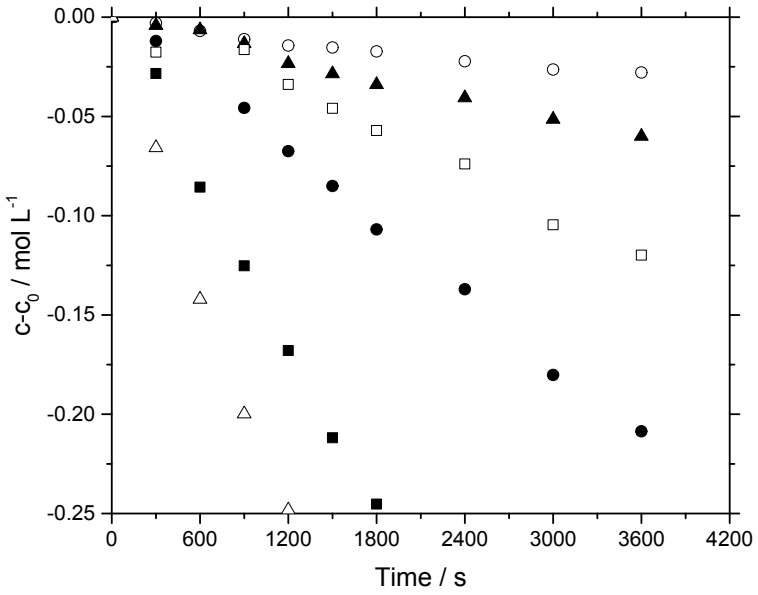

Figure S9. Integral analysis of toluene hydrogenation using Pd-SCILL-**2** catalysts. Temperatures as indicated in Figure S5.

Agitation speed variation

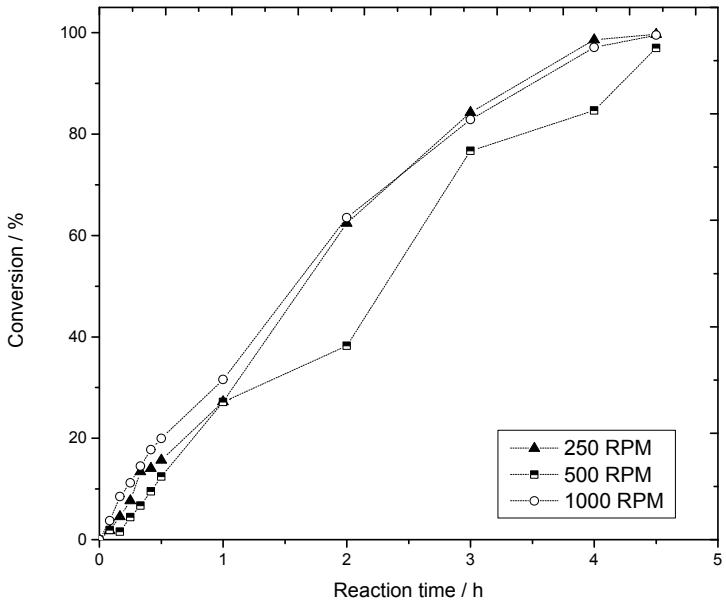

Figure S10. Conversion over time plot for the agitation speed variation of the hydrogenation of toluene using Pd/C catalyst. Reaction conditions: $p_{hydrogen}$ = 15 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 250-1000 min^{-1}.

Metal leaching studies

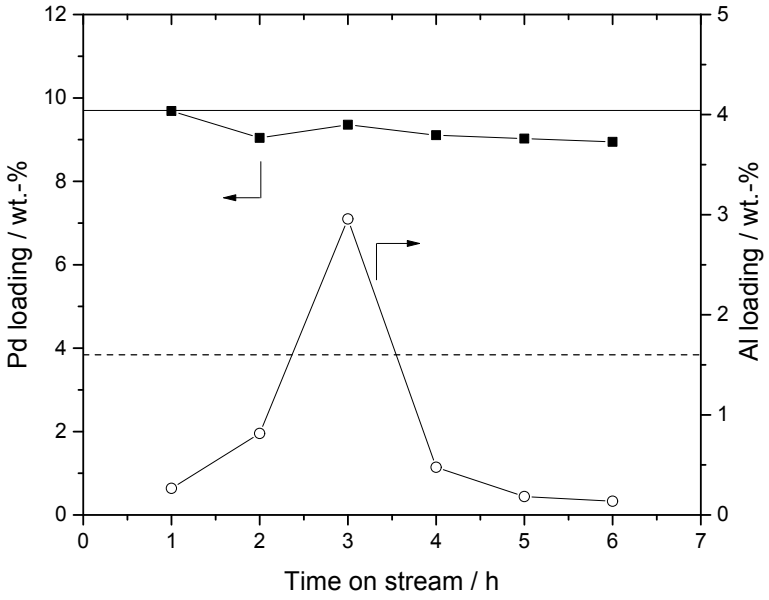

Figure S11. Leaching studies determined via ICP analysis of the Pd-SCILL samples. Reaction conditions: T = 60 °C, $p_{hydrogen}$ = 1 bar, $c_{toluene}$ = 0.25 mol L^{-1}, solvent = 100 mL cyclohexane, m_{cat} = 1 g, w_{Pd} = 10 wt%, stirring speed = 1000 min^{-1}, ionic liquid coating = 13 wt%. The solid line indicates the initial Pd loading, the dashed line indicates the initial Al loading.