Electronic Supplementary Material (ESI) for RSC Sustainability.

Tailoring lixiviant properties to optimise selectivity in E-waste recycling

Jennifer M. Hartley,[a]* Sean Scott,[a] Rodolfo Marin Rivera,[a] Phil Hunt,[a] Anthony J. Lucio,[a] Philip Bird,[b] Robert Harris,[a] Gawen R. T. Jenkin,[b] Andrew P. Abbott [a]

[a] *School of Chemistry, University of Leicester, Leicester, LE1 7RH, UK*

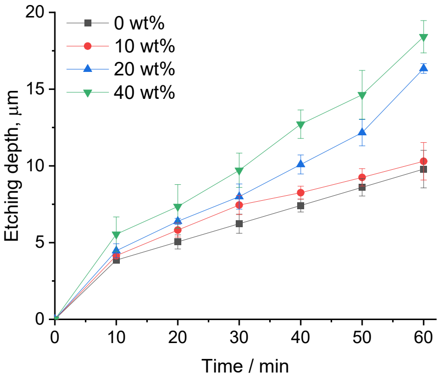
[b] *School of Geography, Geology and the Environment, University of Leicester, Leicester, LE1 7RH, UK*

* jmh84@le.ac.uk

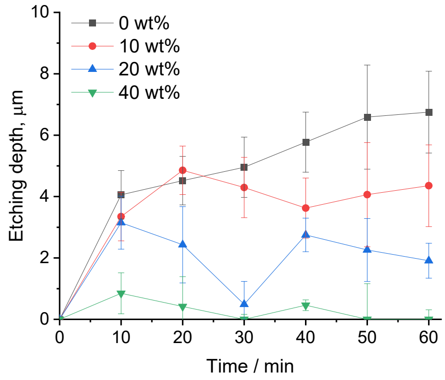
Supplementary Information

Figure S1: Resin block containing the wires used for etching experiments. Wires are circled to show them up against the dark background.

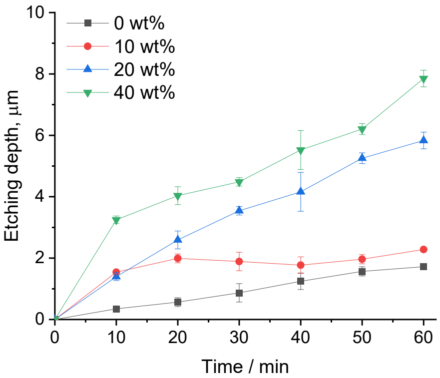
a) Copper



b) Silver



c) Gold



d) Nickel

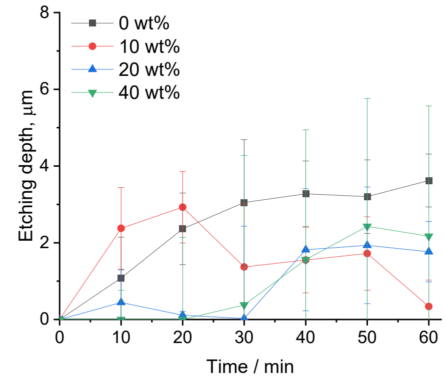


Figure S2: Etching rates for a) copper, b) silver, c) gold, and d) nickel wires over the course of 60 minutes in EG: ChCl containing a nominal concentration of 0.1 mol kg^{-1} iodine at 50 °C and as a function of water content. Lines are included to guide the eye.

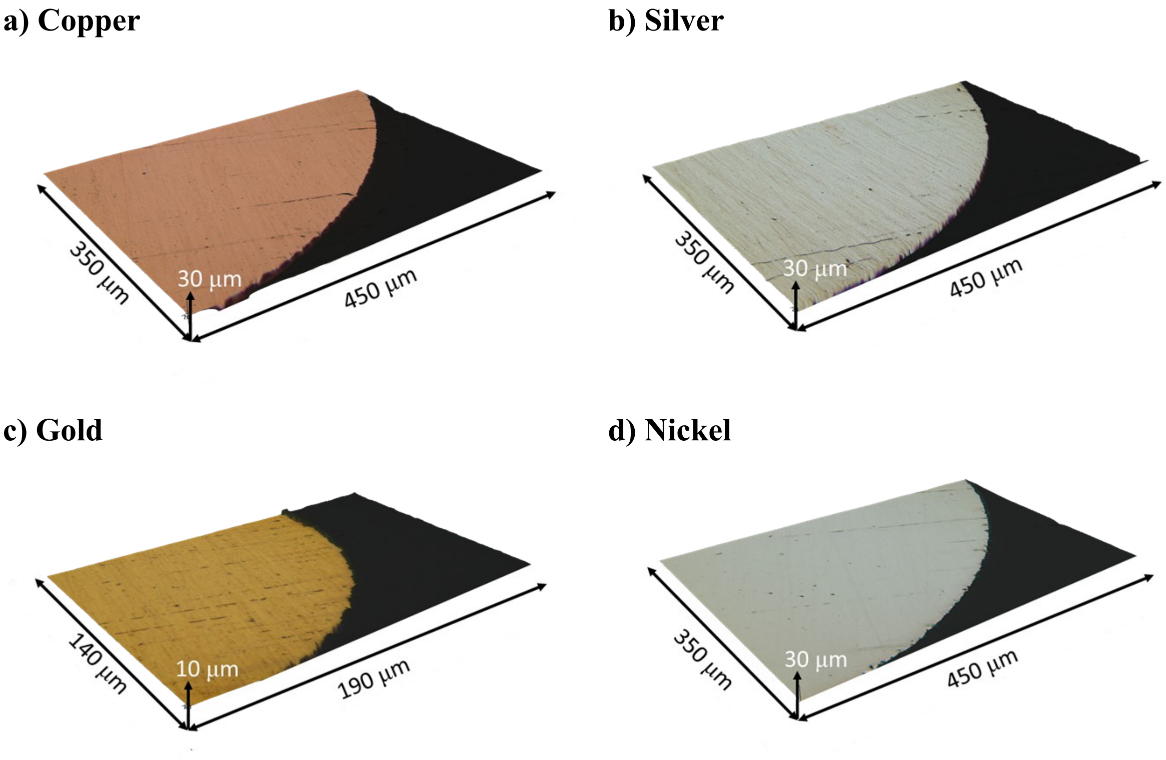


Figure S3: 3DM images of the metal wires before etching: a) copper, b) silver, c) gold, and d) nickel. Images recorded at 20x magnification (Cu, Ag, Ni) and 50x magnification (Au).

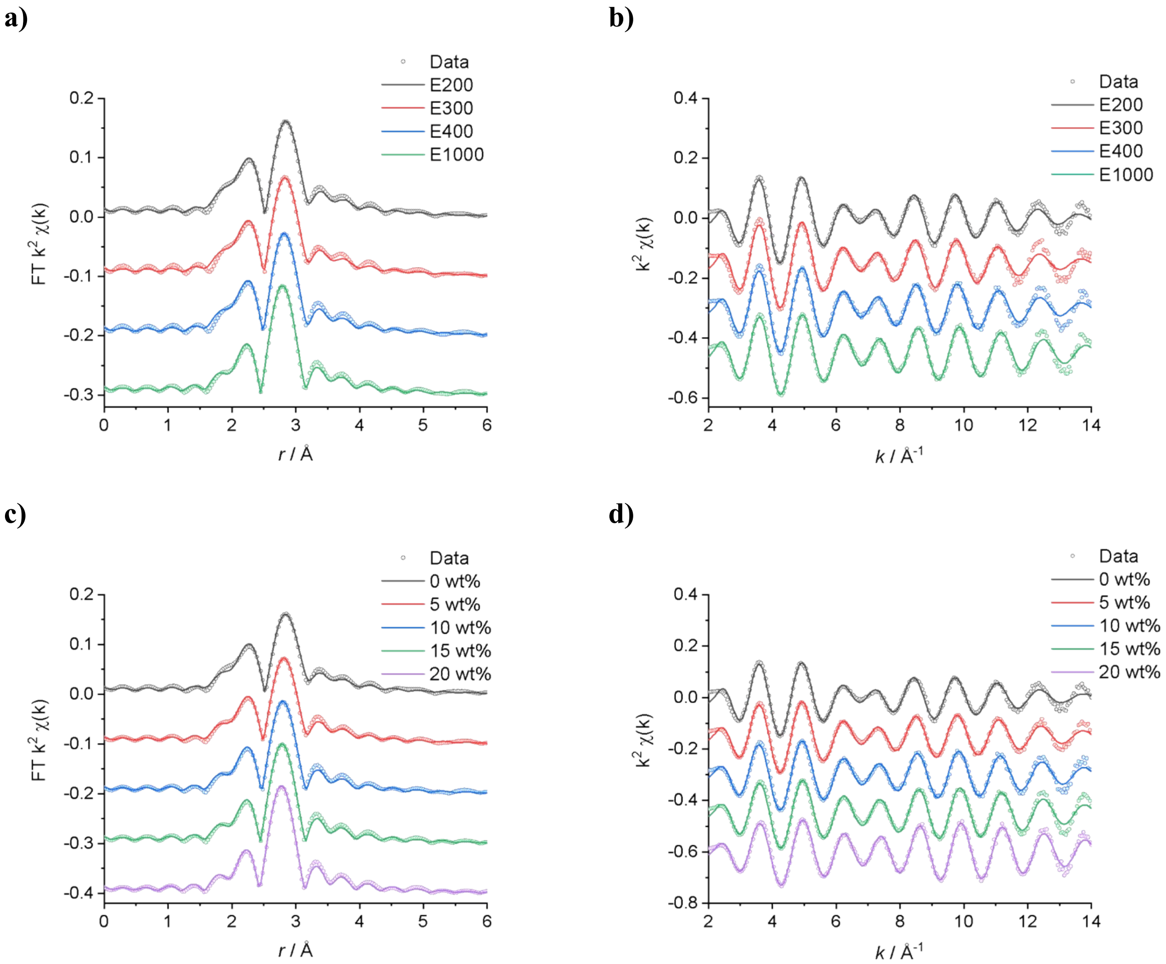


Figure S4: Fourier transforms (a, c) and k^2-weighted EXAFS (b, d) of solutions containing nominally 0.1 mol kg^{-1} iodine in EG: ChCl, with respect to ethylene glycol content (top) and water content (bottom).

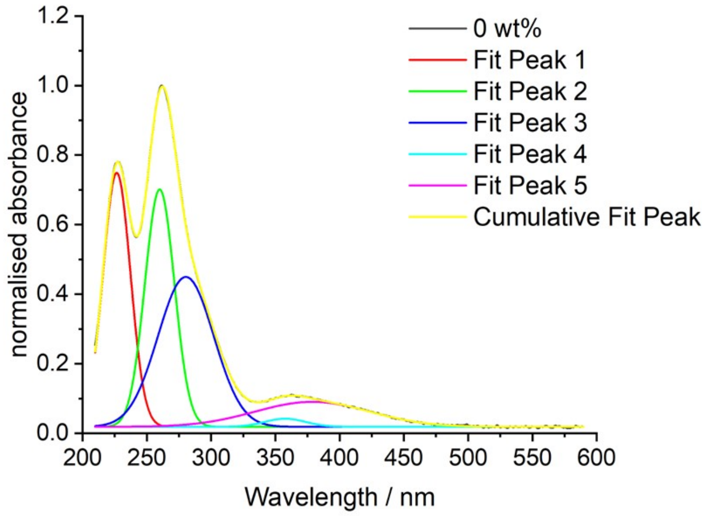


Figure S5: Example of the peak fitting process using 0 wt% water in EG: ChCl. The Origin "multiple peak fitting" function was used.

Table S1: Molality of chloride, EG, and water in the different systems investigated, along with solvent viscosity values and the diffusion coefficient for the $[X_3]^-$ trihalide species (where X = iodine or chloride).

	ChCl / mol kg^{-1}	**EG / mol kg^{-1}**	**H_2O / mol kg^{-1}**	**Viscosity / mPa s**	**D$[X_3]^-$ / cm^2 s^{-1}**
0 wt% = EG: ChCl 2:1	3.8	7.6	/	38 [a]	7.82 x 10^{-8} [c]
10 wt%	4.4	6.8	5.6	29.1 [b]	2.98 x 10^{-7} [c]
20 wt%	3.0	6.1	11.1	19.8 [b]	1.68 x 10^{-6} [c]
30 wt%	2.7	5.3	16.7	13.3 [b]	2.36 x 10^{-6} [c]
40 wt%	2.3	4.5	22.2	11.2 [b]	3.00 x 10^{-6} [c]
100 wt%	/	/	55.6	1	n.a.
EG: ChCl 3:1	3.1	9.2	/	27 [a]	n.a.
EG: ChCl 4:1	2.6	10.3	/	20 [a]	n.a.
EG: ChCl 10:1	1.3	13.1	/	17 [a]	n.a.

[a] *Harris, 2005*. Temperature = 20 °C
[b] *Al-Murshedi et al., 2019*. Temperature = 35 °C
[c] *Al-Murshedi, 2018*. Temperature = 35 °C

Table S2: EXAFS fitting parameters for solutions of 0.1 mol kg^{-1} iodine in EG: ChCl with varying water contents. All fits were made using transmission data. Errors are presented in brackets after the fitted values.

Water content / wt%	**Coordinating atom/group**	**Number of atoms, *N***	**Distance from I, *r* (Å)**	**Debye-Waller factor, *a* (Å^2)**	**Fit index**	**Proposed species**
0 [c]	Cl	0.25(7)	2.546(8)	0.003(2)	0.0043	$3[I_2Cl]^- : 2[I_3]^-$
	I	1.4(2)	2.801(6)	0.011(1)		
5	Cl	0.22(6)	2.55(1)	0.003(2)		$3[I_2Cl]^- : 2[I_3]^-$ + trace I_2
	I	1.3(1)	2.778(5)	0.010(1)		
10	Cl	0.20(6)	2.54(2)	0.003(2)		$3[I_2Cl]^- : 2[I_3]^-$ + trace I_2
	I	1.2(2)	2.765(7)	0.009(1)		
15	Cl	0.16(5)	2.54(1)	0.003(2)		$3[I_2Cl]^- : 2[I_3]^-$ + significant I_2
	I	1.2(1)	2.757(4)	0.0078(7)		
20	Cl	0.15(6)	2.54(2)	0.003(2)		$[I_2Cl]^- : I_2$
	I	1.1(1)	2.750(6)	0.0065(9)		

[d] Spectrum is the same as in *Hartley et al., 2022*. Small differences in fitted values are due to the series fitting models used. Both fits are within the error of each other.

Table S3: EXAFS fit parameters for solutions of 0.1 mol kg^{-1} iodine in EG: ChCl with varying ethylene glycol ratios. All fits were made using transmission data. Errors are presented in brackets after the fitted values.

EG: ChCl ratio	Coordinating atom/group	Number of atoms, *N*	Distance from I, *r* (Å)	Debye-Waller factor, *a* (Å^2)	Fit index	Proposed species
2:1 *	Cl	0.4(1)	2.547(9)	0.007(4)	0.0054	3[I_2Cl]$^-$: 2[I_3]$^-$
	I	1.2(1)	2.791(4)	0.010(1)		
3:1	Cl	0.3(2)	2.55(2)	0.005(6)		3[I_2Cl]$^-$: 2[I_3]$^-$
	I	1.3(3)	2.791(7)	0.010(2)		
4:1	Cl	0.3(2)	2.55(2)	0.006(7)		3[I_2Cl]$^-$: 2[I_3]$^-$
	I	1.2(3)	2.782(6)	0.010(2)		
10:1	Cl	0.1(1)	2.53(2)	0.001(6)		1[I_2Cl]$^-$: 3[I_3]$^-$ + trace I_2
	I	1.3(2)	2.761(6)	0.009(2)		

* Note that the 2:1 ratio is the same data as the 0 wt% water content sample. The small variations in fitted values are due to the series fitting model used. However, all fitted values are within the error bars of each other.

Table S4: Peak fitted absorbance values for the UV-vis spectra of iodine in EG: ChCl with different water contents.

Water content / wt%	Absorbances / nm	Proposed species ratio
0	227, 260, 280, 358, 379	3[I_2Cl]$^-$: 2[I_3]$^-$
5	226, 260, 280, 358, 378	3[I_2Cl]$^-$: 2[I_3]$^-$
10	226, 260, 279, 357, 379	3[I_2Cl]$^-$: 2[I_3]$^-$
15	226, 260, 279, 357, 379	3[I_2Cl]$^-$: 2[I_3]$^-$
20	226, 259, 278, 354, 402	3[I_2Cl]$^-$: 2[I_3]$^-$
30	226, 259, 279, 356, 406	2[I_2Cl]$^-$: 1[I_3]$^-$
40	224, 258, 278, 354, 407	2[I_2Cl]$^-$: 1[I_3]$^-$
50	223, 258, 277, 352, 405	2[I_2Cl]$^-$: 1[I_3]$^-$

Table S4: Peak fitted absorbance values for the UV-vis spectra of iodine in EG: ChCl with different EG ratio contents.

Water content / wt%	Absorbance / nm	Proposed species ratio
2:1 *	227, 260, 280, 358, 379	$3[I_2Cl]^- : 2[I_3]^-$
3:1	227, 260, 282, 358, 381	$3[I_2Cl]^- : 2[I_3]^-$
4:1	226, 260, 282, 357, 384	$3[I_2Cl]^- : 2[I_3]^-$
10:1	226, 260, 282, 357, 394	$3[I_2Cl]^- : 2[I_3]^-$
* Note that the 2:1 ratio is the same data as the 0 wt% water content sample.		

References

[a] R. C. Harris, *Physical properties of alcohol based deep eutectic solvents*, University of Leicester, 2008.

[b] A. Y. M. Al-Murshedi, J. M. Hartley, A. P. Abbott and K. S. Ryder, *Transactions of the IMF*, 2019, **97**, 321-329.

[c] A. Y. M. Al-Murshedi, *Deep eutectic solvent-water mixtures*, University of Leicester, 2018.

[d] J. M. Hartley, S. Scott, Z. Dilruba, A. J. Lucio, P. J. Bird, R. C. Harris, G. R. T. Jenkin and A. P. Abbott, *Phys. Chem. Chem. Phys.*, 2022, DOI: 10.1039/D2CP03185J.