Application of Switchable Hydrophilicity Solvents to the recycling of multilayer packaging materials

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Table S1. Cradle-to-gate inventory for the disposal of 1 ton of composite packaging into landfill.

Landfill scenario	***Amount***	***Unit***
Input process		
Coal, hard, 30.7 MJ/kg	301.0	kg
Electricity, medium voltage, at grid (China)	0.4	MWh
Avoided process		
Kraft paper, unbleanched, at plant	660.0	kg
Output process		
Disposal, PE, 0.4% water, to sanitary landfill	200.0	kg
Disposal, aluminium, 0% water, to sanitary landfill	50.0	kg
Disposal, paper, 11.2% water, to sanitary landfill	90.0	kg

Table S2. Cradle-to-gate inventory for the recovery of 1 ton of composite packaging with formic acid treatment.

Formic acid scenario	***Amount***	***Unit***
Input process		
Coal, hard, 30.7 MJ/kg	301.0	kg
Diesel, at refinery	3.4	kg
Electricity, medium voltage, at grid (China)	0.6	MWh
Formic acid, at plant	39.3	kg
Avoided process		
Alluminium, primary, at plant	36.0	kg
Polyethylene, LDPE, granulate, at plant	196.0	kg
Kraft paper, unbleanched, at plant	660.0	kg
Output process		
Disposal, PE, 0.4% water, to sanitary landfill	4.0	kg
Disposal, aluminium, 0% water, to sanitary landfill	14.0	kg
Disposal, paper, 11.2% water, to sanitary landfill	90.0	kg

Table S3. Cradle-to-gate inventory for the recovery of 1 ton of composite packaging through pyrolysis.

Pyrolysis scenario *	***Amount***	***Unit***
Input process		
Electricity, medium voltage, at grid (China)	1.6	MWh
Output process **		
Heat, waste	9.5E-01	MWh
Acetaldehyde	3.1E-06	kg
Benzo(a)pyrene	3.1E-08	kg
Benzene	1.2E-03	kg
Butane	2.2E-03	kg
Methane, fossil	6.2E-03	kg
Carbon monoxide, fossil	6.5E-03	kg
Carbon dioxide, fossil	1.7E+02	kg
Acetic acid	4.7E-04	kg
Formaldehyde	3.1E-04	kg
Mercury	9.3E-08	kg
Dinitrogen monoxide	3.1E-04	kg
Nitrogen oxides	5.6E-02	kg
PAH, polycyclic aromatic hydrocarbons	3.1E-05	kg
Particulates, < 2.5 um	6.2E-04	kg
Pentane	3.7E-03	kg
Propane	6.2E-04	kg
Propionic acid	6.2E-05	kg
Sulfur dioxide	1.7E-03	kg
Dioxin, 2,3,7,8 Tetrachlorodibenzo-p-	9.3E-14	kg
Toluene	6.2E-04	kg
Waste water - untreated, slightly organic and anorganic contamined EU-27 S	328.0	kg
Bitumen to HA chemical landfill	11.0	kg
Disposal, PE, 0.4% water, to sanitary landfill	113.0	kg
Disposal, aluminium, 0% water, to sanitary landfill	2.0	kg
Avoided process		
Alluminium, primary, at plant	68.0	kg
Polyethylene, LDPE, granulate, at plant	187.0	kg
Hard coal briquettes, at plant	1.3	MWh
Electricity, medium voltage, at grid (China)	0.9	MWh

* all the input and output were evaluated using the following packaging composition: 63% paper, 30% LDPE and 7% Al. According with average composition the amount of recovered Al and LDPE are estimated around 49 and 125 kg per t treated. On the other hand, the quantity dumped is 3 and 75 kg respectively.

** emissions derived from the combustion of the CO/H_2 fraction and assumed to be equal to the emission of methane burned in furnace.

Table S4. Cradle-to-gate inventory for the recovery of 1 ton of composite packaging through switchable solvent.

SHS scenario	*Amount*	*Unit*
Input process		
Electricity, medium voltage, at grid (China)	0.2	MWh
Heat, unspecific, in chemical plant	0.1	MWh
Water, groundwater consumption	50	kg
Coal, hard, 30.7 MJ/kg	301.0	kg
CO_2*	0.6	kg
DMCHA**	1.0	kg
Output process		
Waste water - untreated, slightly organic and anorganic contamined EU-27 S	2.6E-02	kg
Disposal, PE, 0.4% water, to sanitary landfill	30.0	kg
Disposal, aluminium, 0% water, to sanitary landfill	0.5	kg
Disposal, paper, 11.2% water, to sanitary landfill	90.0	kg
Avoided process		
Alluminium, primary, at plant	42.6	kg
Alluminium oxide, at plant	6.9	kg
Polyethylene, LDPE, granulate, at plant	170.0	kg
Kraft paper, unbleanched, at plant	660.0	kg

* obtained from air using GWP value reported in the literature.[1]

** DMCHA is not reported in software libraries; Finechem tool [2,3] was used to evaluate the carbon footprint due to its synthesis.

Figure S1. Contribution of each category to the cumulative score for the recovery treatments only (landfill not included).

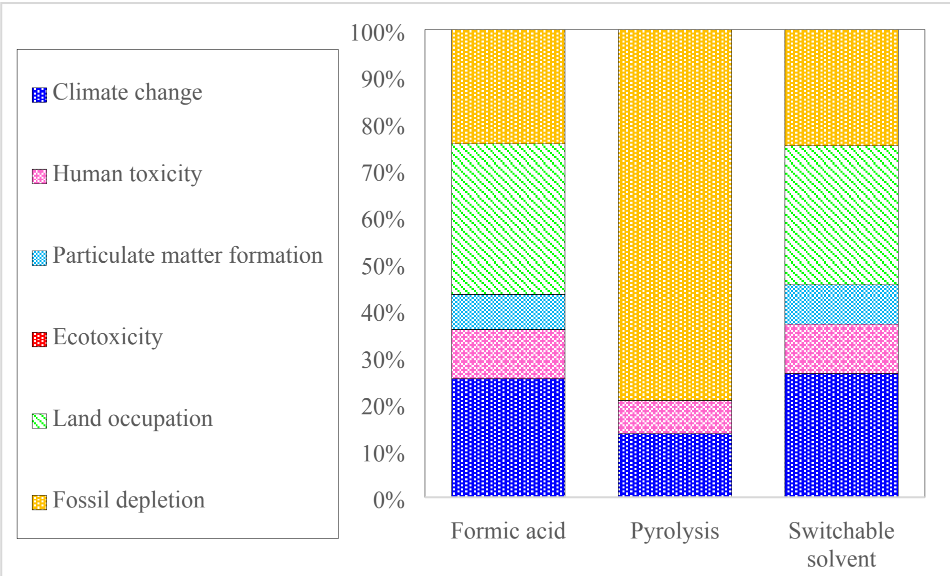

Figure S2. Network tool for ***a***) the FD and ***b***) CC categories, SHS-route.

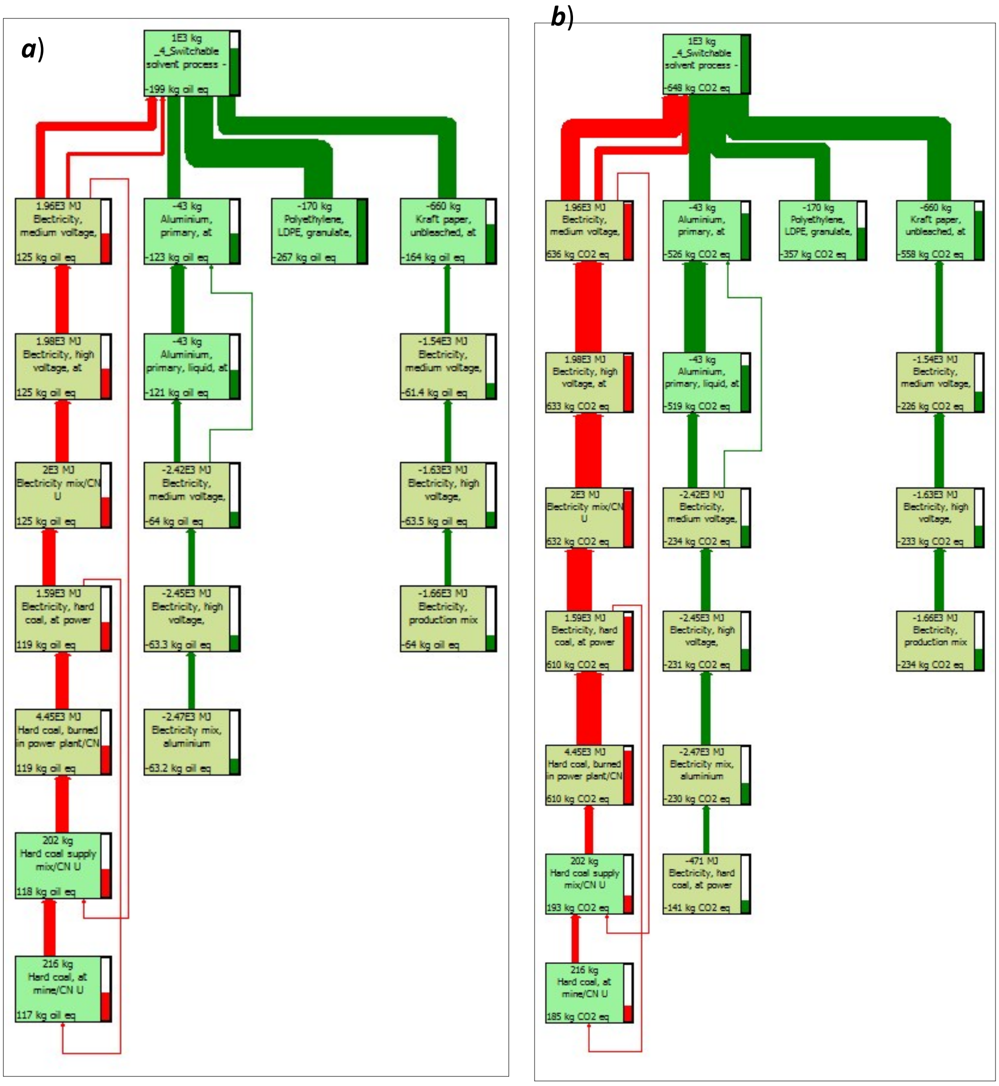

Table S5. Inventory of the avoided substances released per PMF and HT categories.

	Contribution
<u>PMF</u>	
NOx	-37%
PM2.5-10μm	-34%
PM<2.5μm	-26%
SO_2&NH_3	-3%
<u>HT</u>	
Pb	-21%
V	-18%
As	-17%
Mn	-13%

1 N. von der Assen, P. Voll, M. Peters and A. Bardow, *Chem. Soc. Rev*., 2014, **43**, 7982.

2 G. Wernet, S. Hellweg, U. Fischer, S. Papadokonstantakis and K. Hungerbühler, *Environ. Sci. Technol*., 2008, **42**, 6717.

3 G. Wernet, S. Papadokonstadakis, S. Hellweg and K. Hungerbühler, *Green Chem*., 2009, **11**, 1826.