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# Supporting Information

## High-value utilization of recovered $LiPF_6$ from retired lithium-ion batteries

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**Table S1.** The possible hazards caused by each component of the electrolyte.

| Species | Materials | Main chemical properties | Potential environmental hazards |
|---|---|---|---|
| Lithium salt | $LiPF_6$ | Has high corrosivity and can decompose in contact with water to produce HF, react with strong oxidants, and burn to produce toxic substances such as $P_2O_5$ | Cause fluorine pollution and raise pH of environment |
| | $LiBF_4$ | Has high corrosivity, reacts violently with water and acid to produce HF gas, and produces $Li_2O$, $B_2O_3$ and other harmful substances when burned or decomposed by heat | Cause fluorine pollution and raise pH of environment |
| | $LiClO_4$ | Reacts with strong reducing agents, nitromethane and hydrazine violently; Combusts and produces LiCl, $O_2$ and $Cl_2$ | Toxic gas |
| | $LiAsF_6$ | Soluble in water, strong hygroscopicity, reacts with acid to produce toxic gases HF, arsenic compounds | Fluorine pollution and arsenic pollution |
| | $LiCF_3SO_3$ | Combusts and produces CO, $CO_2$, $SO_2$, HF; Reacts with oxidants and strong acids to produce HF | Fluorine pollution, toxic gases and acid rain |
| Electrolyte solvent | Ethylene carbonate (EC) | Reacts with acid, alkali, strong oxidant and reducing agent, combust to produce CO and $CO_2$, and hydrolyzes to produce aldehyde and acid | Aldehyde and organic acid pollution |
| | Propylene carbonate (PC) | Reacts with water, air and strong oxidants, combusts to produce CO and $CO_2$; Thermal decomposition will produce harmful gases such as aldehyde des and ketones | Aldol and ketone organic pollution |
| | Dimethyl carbonate (DMC) | Interacts with water to form strong alkali and can react with substances such as oxygen, nitrogen, carbon dioxide and acids | Organic pollution such as methanol |
| | Diethyl carbonate (DEC) | Reacts violently with water, strong oxidants, strong acids, strong alkalis and strong reducing substances, and combusts to produce CO and $CO_2$ | Organic pollution such as alcohol |
| | Ethylene glycol dimethyl ether (DME) | Flammable and explosive; Reacts with water, strong alkali, and strong oxidizing reducing agent, and easily forms explosive peroxides when exposed to light or heat | Organic pollution such as methanol |

| | | |
|---|---|---|
| 1-ethoxy-2-(2-ethoxyethoxy)ethane (DEE) | Flammable and explosive, easy to form explosive peroxides in the presence of fire, light or heat, and react violently with strong acids and strong oxidants | Organic pollution such as alcohol |
| Ethyl Methyl Carbonate (EMC) | Reacts with water, strong acid, alkali, and strong oxidant, and the hydrolyzate has methanol, which is flammable | Organic pollution such as alcohol |
| Ethyl acetate (EA) | Reacts with chlorosulfonic acid, lithium aluminum hydride, fuming sulfuric acid and other substances, it will decompose in contact with water or moisture, burn or decompose in contact with fire and heat, and produce toxic gases such as CO | Organic acid pollution |
| Gamma-butyrolactone (GBL) | Reacts violently with strong oxidants, strong acids and strong alkalis, and combusts to produce harmful gases such as CO, $CO_2$, and NO | Alcohol, acid organic pollution |

**Synthesis of DTMSO**

The synthesis of DTMSO needs to be carried out under anhydrous conditions, due to the fact that DTMSO is easily hydrolyzed into oxalic acid when meeting $H_2O$. Firstly, anhydrous oxalic acid, chlorotrimethylsilane and HMDS are dispersed in an anhydrous DMC solvent with the stoichiometric ratio of 3:2:2. After reaction at 75 ℃ for 6 h under the condition of air isolation, the insoluble matter is filtered off, and the filtrate is distilled by vacuum distillation to remove the solvent. Finally, white needle-shaped DTMSO crystals are obtained. The yield is more than 65%, with the purity of 99.1%. The TG – DTA, $^{11}$C NMR and $^{1}$H NMR spectra of the prepared DTMSO are shown in Fig. S1. It can be seen that the thermal decomposition temperature is 131.1 ℃, the characteristic peaks of $^{11}$C NMR are located at 161.40, -0.08 ppm, and the characteristic peaks of $^{1}$H NMR are located at 0.33 ppm.

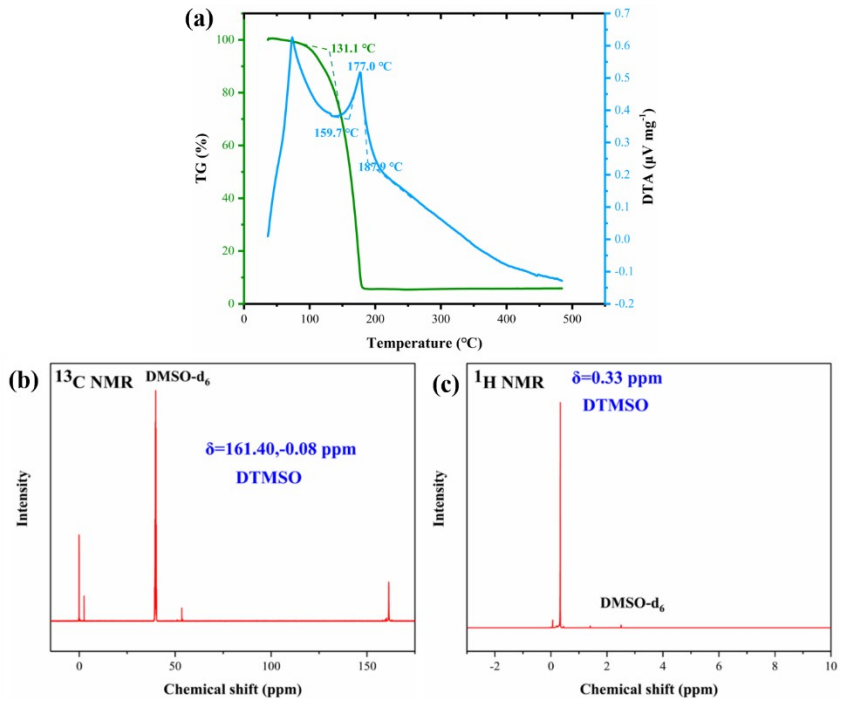


**Fig. S1.** Characterizations of the prepared DTMSO (a) TG - DTA curves; (b and c) $^{11}C$ NMR and $^{1}H$ NMR spectroscopies.

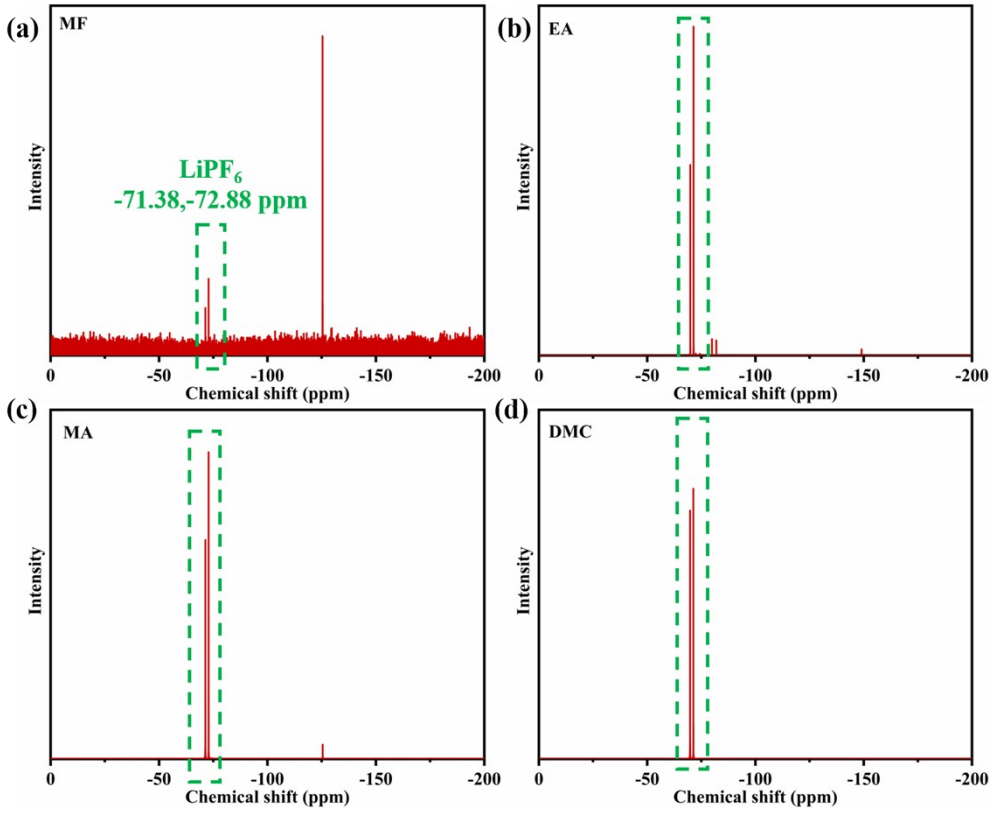


**Fig. S2.** $^{19}F$ NMR spectra of electrolytes obtained by different leaching agents from

retired LIBs: (a) methyl formate (MF); (b) ethyl acetate (EA); (c) methyl acetate (MA); (d) DMC.