Supplementary Information

Coordination Chemistry in magnesium battery electrolytes: how ligands affect their performance

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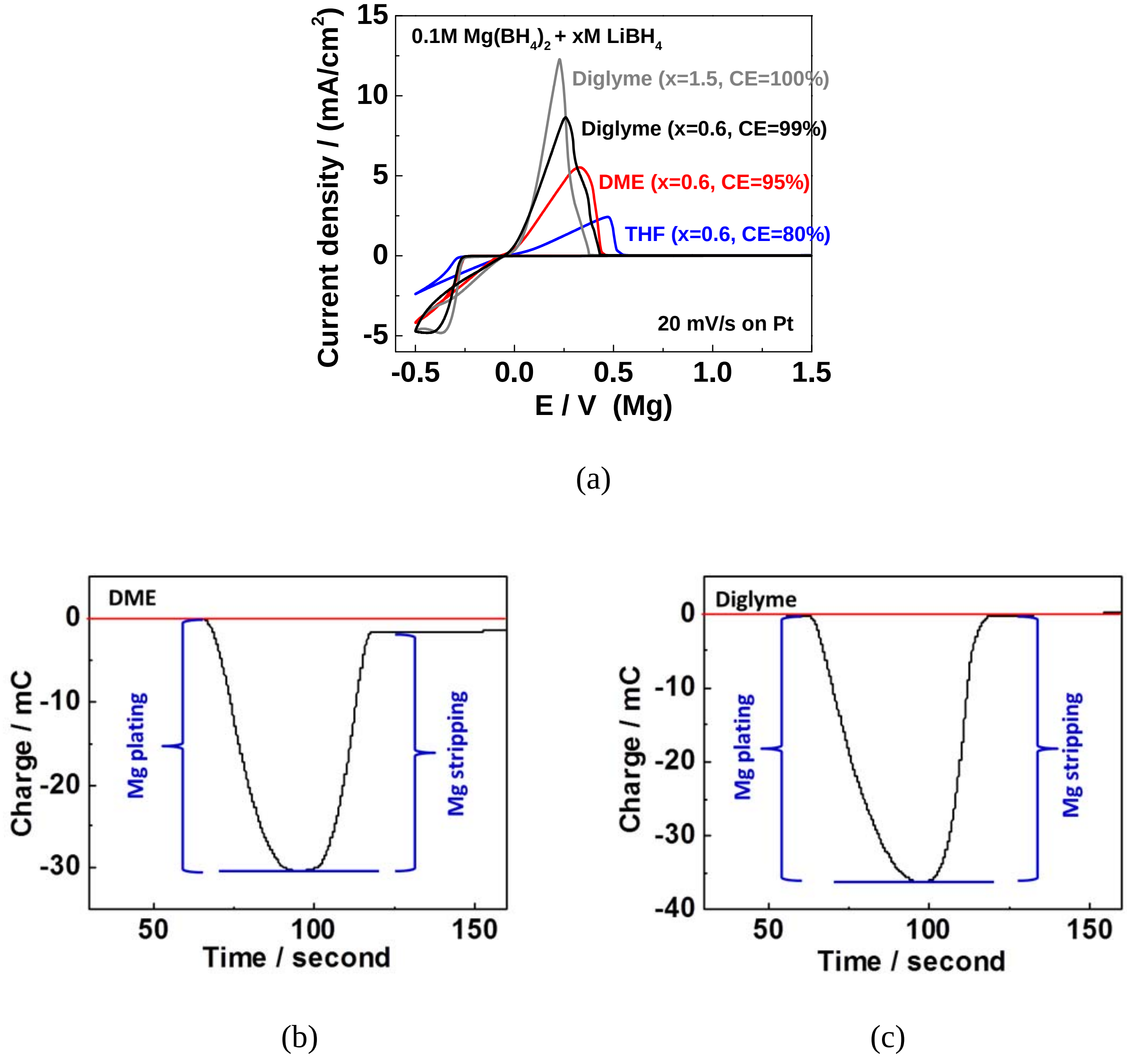

(a)

(b)

(c)

Figure S1. (a) CVs recorded on Pt electrodes in the electrolytes by dissolving $Mg(BH_4)_2/LiBH_4$ in diglyme, DME, and THF. Diglyme shows much better performance (higher current density, 100% coulombic efficiency). (b, c) The charge vs time curves on Pt electrode during Mg plating/stripping in 0.1M $Mg(BH_4)$-0.6M $LiBH_4$/DME (b) and 0.1M $Mg(BH_4)_2$-1.5M $LiBH_4$/Diglyme (c); The curves show the coulombic efficiency of 95% (b) and 100% (c) for 0.1M $Mg(BH_4)_2$-1.5M $LiBH_4$/Diglyme and 0.1M $Mg(BH_4)$-0.6M $LiBH_4$/DME respectively.

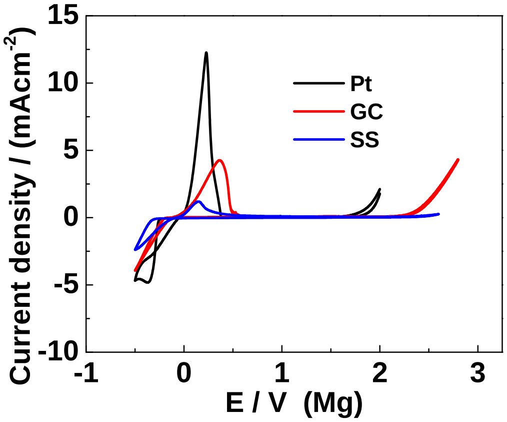

Figure S2. CVs recorded on Pt, glass carbon (GC) and stainless steel (SS) electrodes in the electrolyte, $Mg(BH_4)_2$-$LiBH_4$-DGM ([$LiBH_4$]=1.5 M). On GC and SS, anodic stability is observed over 2.0V (vs Mg/Mg^{2+}).

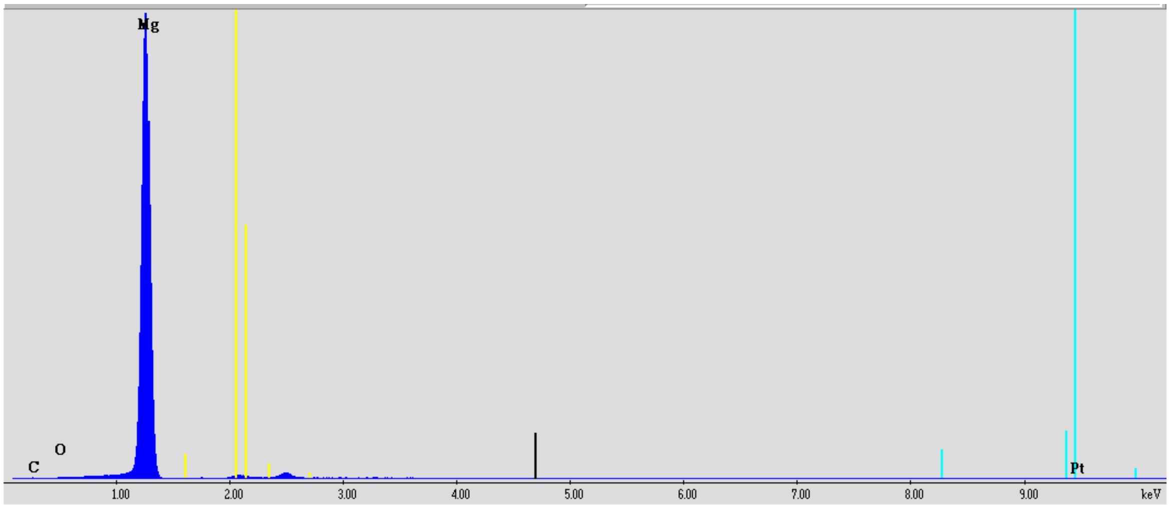

Figure S3. Energy-dispersive X-ray of an Mg sample plated from $Mg(BH_4)_2$-$LiBH_4$-DGM electrolyte with [$LiBH_4$]=1.5M.

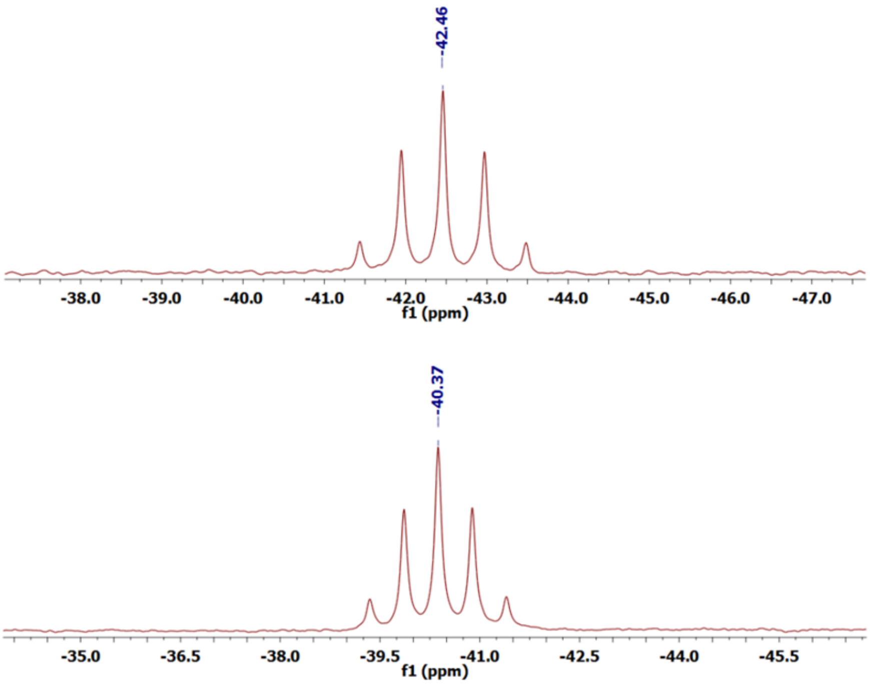

Figure S4. ^{11}B NMR spectra of $\mathbf{Mg(BH_4)_2DGM}$ (a) and $\mathbf{Mg_2(BH_4)_4(DME)_3}$ (b) recorded at 22 °C in CD_2Cl_2. Chemical shift values labeled at the top of resonances.

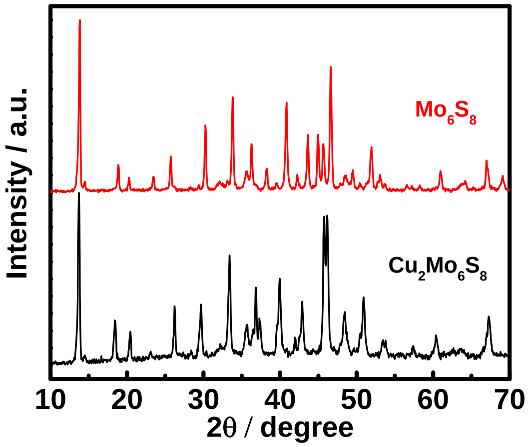

Figure S5. XRD patterns of $Cu_2Mo_6S_8$ and Mo_6S_8 from molten salt synthesis. The XRD patterns are consistent with those in literature.[1]

References:

1 Lancry, E., Levi, E., Mitelman, A., Malovany, S. & Aurbach, D. Molten salt synthesis (MSS) of $Cu_2Mo_6S_8$- new way for large-scale production of chevrel phases. *J. Solid State Chem.* **179,** 1879-1882 (2006).