Electronic Supplementary Information for

Molten Air - A new, highest energy class of rechargeable batteries

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Supplementary Information:
   Carbonate electrolyte stability

Carbonate electrolyte stability. We have recently shown that under many conditions molten lithium carbonate readily absorbs atmospheric carbon dioxide, providing a facile route to decrease CO_2 in the atmosphere. As summarized in the CO_2/carbonate equilibrium diagram in Figure S-1, we now calculate from the known variation of standard enthalpies and entropies with temperature[23-25] that barium carbonate has an even larger affinity for CO_2 capture than lithium carbonate.

The equilibrium curves in the figure summarize the partial pressure of CO_2 and dissolved oxide concentration relative to carbonate in which CO_2 absorption occurs (above the line) or carbonate decomposition occurs (below the line). This equilibrium can be controlled through cation and temperature choice, and the concentration of oxide in the melt. Molten carbonate can gain or lose mass through CO_2 absorption or emission, and the concentration of carbon dioxide maintained above the melt is in accord with the equilibrium:

$$MCO_3 \rightleftharpoons MO + CO_2; \quad M= Li_2, Na_2, K_2, Ba, etc \quad\quad\quad\quad (S\text{-}1)$$

Barium carbonate is solid at lithium carbonate's 723°C melting point. However as summarized in the Figure S-1 inset, barium carbonate readily dissolves in lithium carbonate, and a eutectic comprised of 69% by mass barium to lithium carbonate melts at 609°C.
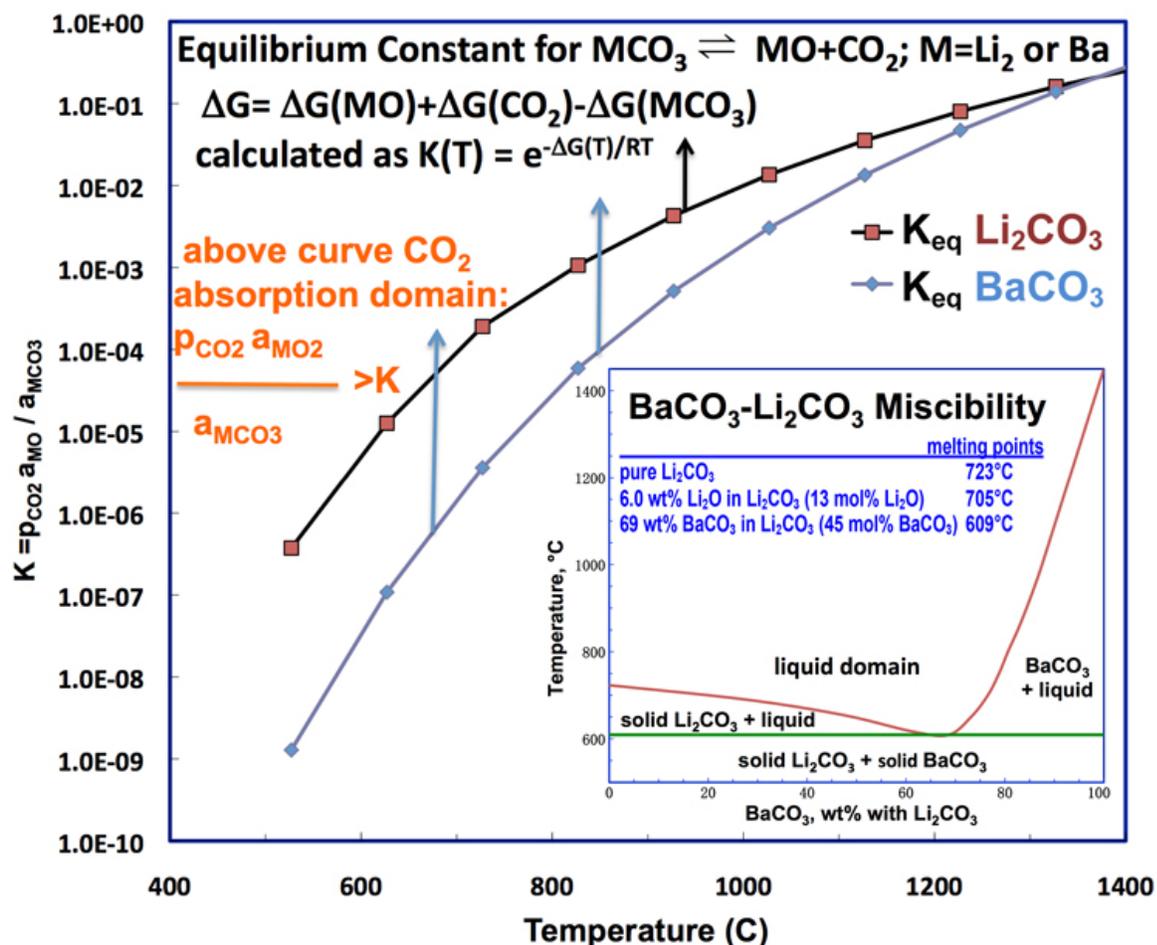
Figure S-1. Comparison of the equilibrium constant for Li_2CO_3 and $BaCO_3$, decomposition or absorption of CO_2 as calculated from the thermochemistry of the carbonate, carbon dioxide and oxide components. Inset: Phase diagram of the $BaCO_3$ - Li_2CO_3 system (100% or 0% respectively indicate pure barium or lithium carbonate); modified from reference *33*. The 705°C Li_2O/Li_2CO_3 mix melting point is noted for comparison, but not shown on the curve.