Supporting Information

Achieving both High Ionic Conductivity and High Interfacial Stability with the $Li_{2+x}C_{1-x}B_xO_3$ Solid-State Electrolyte: Design from Theoretical Calculations

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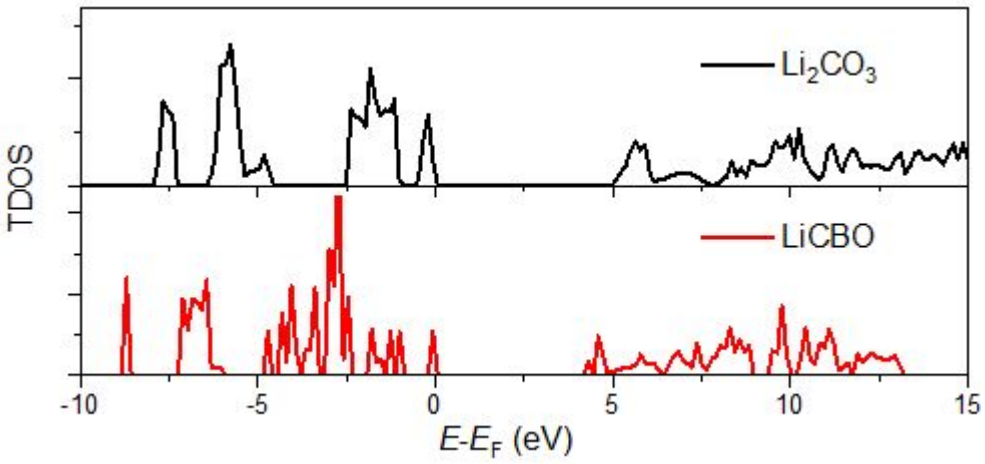

Figure S1. Total density of states for Li_2CO_3 and LCBO (x = 0.375).

Table S1. The phase equilibria at the reduction and oxidation potentials of LCBO.

Potential (V)	Phase equilibria
0	$Li_2O + LiC_{12} + LiBC$
0.12	$Li_2O + LiBC + C$
0.45	$Li_2O + Li_3BO_3 + C$
1.27	$Li_3BO_3 + Li_2CO_3$
3.47	$Li_6B_4O_9 + LiO_8 + Li_2CO_3 + Li$
3.52	$LiBO_2 + LiO_8 + Li_2CO_3 + Li$
3.68	$Li_2B_4O_7 + LiO_8 + Li_2CO_3 + Li$
3.69	$LiO_8 + Li_2CO_3 + Li_3B_7O_{12} + Li$
3.81	$Li_2CO_3 + Li_3B_7O_{12} + O_2 + Li$
4.10	$CO_2 + Li_3B_7O_{12} + O_2 + Li$
4.21	$Li_3B_{11}O_{18} + CO_2 + O_2 + Li$
4.45	$CO_2 + B2O3 + O_2 + Li$

Table S2. The phase equilibria and decomposition energies (maximum absolute value of mutual energy, meV/atom) of the electrolyte-electrode interfaces without any applied chemical potential. Electrodes here represent $LiXO_2$ (X = Co, Mn and Ni), $LiFePO_4$, and $LiMn_2O_4$. *x* represents molar fraction of electrolyte in the reaction of *x*·electrolyte + (1-*x*)·electrode.

Electrode	Electrolyte	*x*		Δ*E*
Electrodes	Li_2CO_3	--	No reaction	0.0
	Li_3BO_3			
$LiXO_2$		--	No reaction	0.0
$LiMn_2O_4$		0.43	$LiBO_2$, Li_2MnO_3, Mn_3O_4	-23.0
$LiFePO_4$		0.5	$LiFeBO_3$, Li_3PO_4	-56.0
	LCBO			
$LiXO_2$		--	No reaction	0.0
$LiMn_2O_4$		0.3	Li_2CO_3, Mn_2O_3, $LiBO_2$, Li_2MnO_3,	-12.0
$LiFePO_4$		0.53	Li_2CO_3, $LiFeBO_3$, Li_3PO_4	-26.0

Table S3. The typical phase equilibria and reaction energies (meV/atom) of the electrolyte-electrode interfaces withy applied chemical potential. Electrodes here represent $LiXO_2$ (X = Co, Mn and Ni), $LiFePO_4$, and $LiMn_2O_4$. *x* represents molar fraction of electrolyte in the reaction of $x\cdot$electrolyte + $(1-x)\cdot$electrode.

Electrode	Electrolyte	μ_{Li}		ΔE
	Li_2CO_3		No reaction	0.0
$LiCoO_2$		-4.0	No reaction	0.0
$LiMnO_2$		-4.0	No reaction	0.0
$LiMn_2O_4$		-4.0	No reaction	0.0
$LiNiO_2$		-4.0	Li, $NiCO_3$, O_2	-96.0
$LiFePO_4$		-4.0	Li, $LiFe(CO_3)_2$, $Li_3Fe_2(PO_4)_3$	-100.0
	Li_3BO_3			
$LiCoO_2$		--	No reaction	0.0
$LiMnO_2$		-4.0	Li, $Li_4Mn_5O_{12}$, $Li_3B_7O_{12}$	-282.0
$LiNiO_2$		-4.0	Li, Ni_3BO_5, O_2	-217.0
$LiMn_2O_4$		-4.0	Li, $Li_4Mn_5O_{12}$, $Li_3B_7O_{12}$	-138.0
$LiFePO_4$		-4.0	Li, $Li_3B_7O_{12}$, Li_3PO_4, Fe_2O_3	-227.0
	LCBO			
$LiCoO_2$		--	No reaction	0.0
$LiMnO_2$		-4.0	Li, Li_2CO_3, $Li_4Mn_5O_{12}$, $Li_3B_7O_{12}$	-23.0
$LiNiO_2$		-4.0	Li, Li_2CO_3, $NiCO_3$, O_2, Ni_3BO_5	-96.0

$LiMn_2O_4$	-4.0	Li, Li_2CO_3, $Li_4Mn_5O_{12}$, $Li_3B_7O_{12}$	-49.0
$LiFePO_4$	-4.0	Li, $LiFe(CO_3)_2$, $Li_3Fe_2(PO_4)_3$, $Li_3B_7O_{12}$, Li_3PO_4, Fe_2O_3	-146.0