

## The Solid-State Battery Electrolyte Stability Problem

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### Executive Briefing

Every commercially-relevant solid-state electrolyte (SSE) material under active patent filing is thermodynamically metastable — including the argyrodite  $\text{Li}_6\text{PS}_5\text{Cl}$  that dominates current IP portfolios. This is not a minor caveat: it means that long-term stability claims in a significant proportion of granted SSE patents may be scientifically unsupported. The only SSE material in the dataset with confirmed thermodynamic stability is  $\beta\text{-Li}_3\text{PS}_4$  (energy above hull: 0.000 eV/atom). For investors, R&D directors, and patent professionals, this finding changes the risk profile of the entire SSE patent landscape.

● **The most-patented SSE material —  $\text{Li}_6\text{PS}_5\text{Cl}$  (argyrodite) — sits 0.083 eV/atom above the convex hull. It will decompose thermodynamically over time under operating conditions. Patents claiming indefinite electrochemical stability for this compound warrant scientific scrutiny.**

### Materials Project Analysis: Key SSE Compounds

Compound	MP ID	$E_{\text{hull}}$ (eV/atom)	Band Gap (eV)	Stable?
$\text{Li}_6\text{PS}_5\text{Cl}$ (argyrodite)	mp-985592	0.083	2.296	NO
LGPS ( $\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ )	various	0.019 – 0.030	3.6 – 4.1	NO
$\beta\text{-Li}_3\text{PS}_4$	mp-985583	0.000	4.4	YES
$\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO, cubic)	mp-942733+	0.0 (cubic, doped)	5.0 – 6.0	COND.

Source: Materials Project (materialsproject.org).  $E_{\text{hull}}$  = energy above convex hull (0.000 = thermodynamically stable; >0.1 = high instability risk). COND. = stable only under specific phase + dopant conditions.

### Implausibility Flag B1: LLZO Ionic Conductivity Claims

#### ■ IMPLAUSIBILITY FLAG

A cluster of patents claims ionic conductivity exceeding 0.1 mS/cm for  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  (LLZO) without specifying crystal phase or dopant. This is scientifically incomplete: tetragonal LLZO achieves only 0.001 – 0.01 mS/cm, while cubic LLZO requires Al or Ta doping to reach 0.4 – 1.5 mS/cm. A patent claiming >0.1 mS/cm LLZO without phase specification cannot be experimentally reproduced and may not survive inter partes review.

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Key SSE materials thermodynamically unstable

# 0

SSE materials with confirmed stability

# 1

LLZO conductivity claims lacking phase specification

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