

# Mathematical modelling for the next-generation all-solid-state battery: Nucleation interface

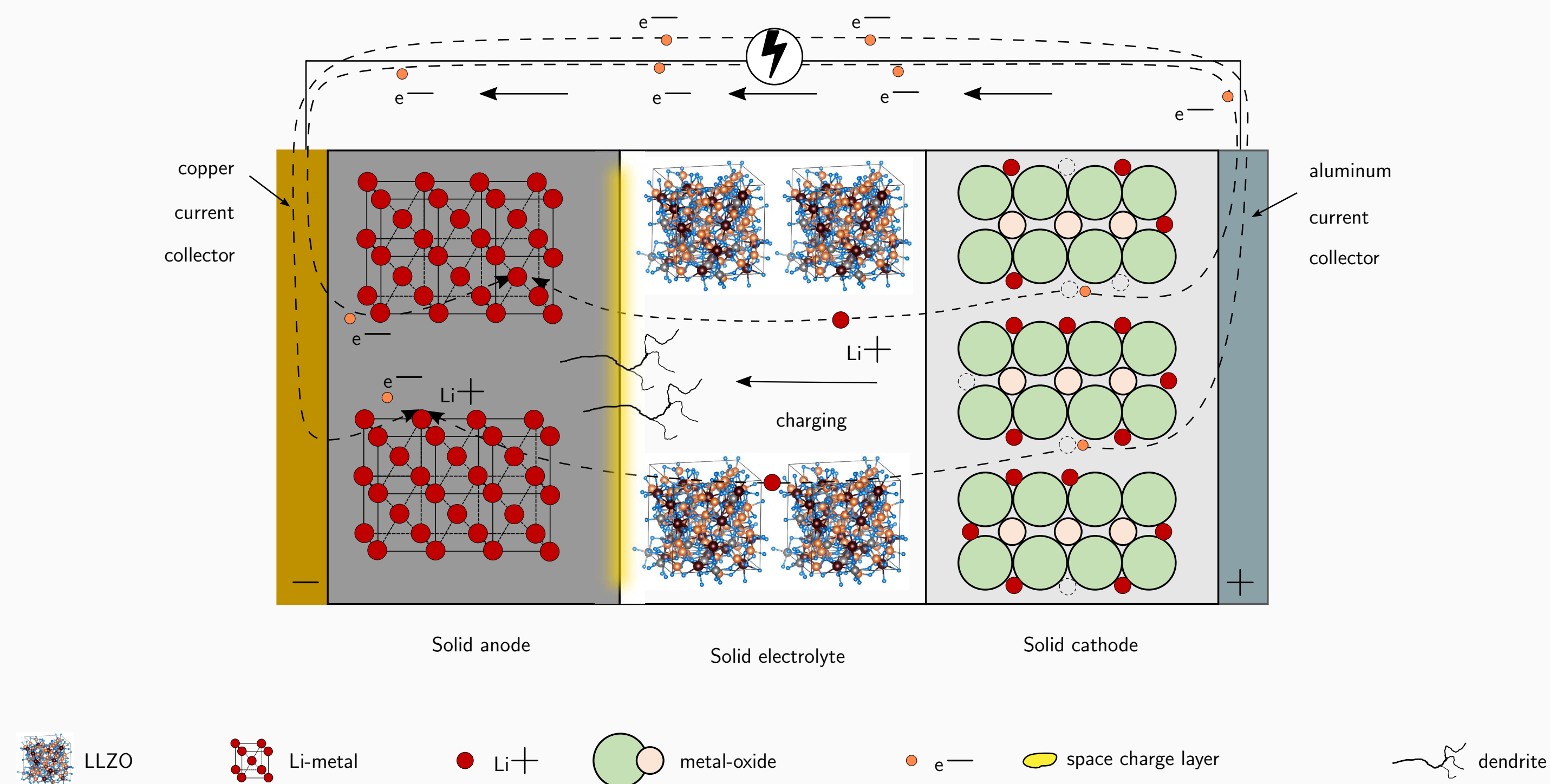
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## Next-generation All-solid-state battery

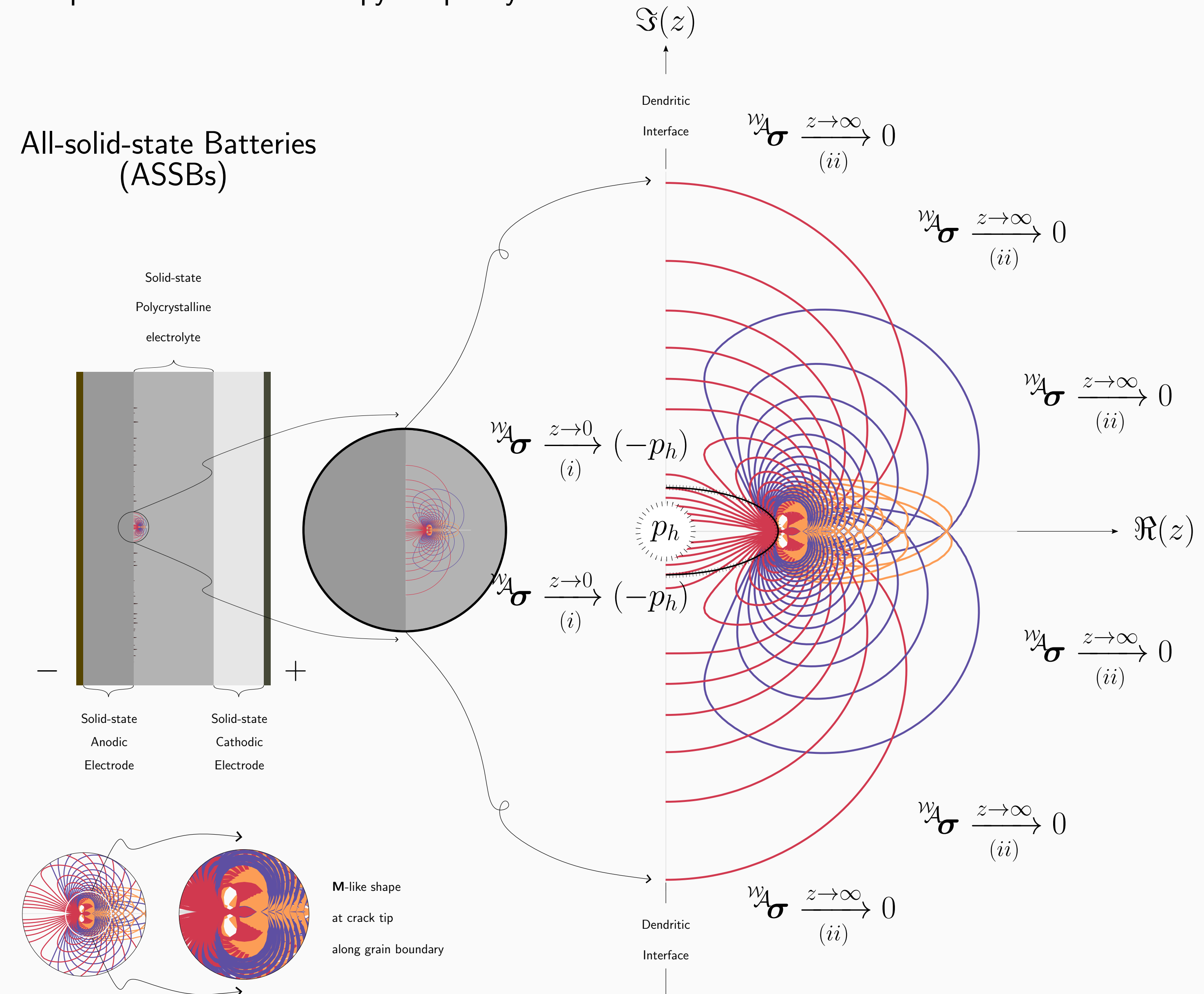
Rechargeable Lithium-ion battery (LIB) stays at the heart of every energy storage system and electric vehicle. Undoubtedly, LIB benefits human life efficiently as well as friendly-environment. Besides, a more advanced LIB, so-called **all-solid-state battery** (ASSB), is introduced recently as ASSB is expected with non-inflammation and non-explosion as seen in common LIBs. Yet, defect due to polarization is one natural phenomenon of **solid electrolyte** (SE) to be tackled.

This poster is aimed to model the polarized SE with the use of **structural tensor**. A typical LIB includes three main components: cathode, anode and electrolyte. Different types of LIB have a variation of constitutive material composed of battery. An ASSB means that the three main components are **all made of solid material**.



## Mathematical model

**Constitutive equation** is first derived from considering local balance laws and enforcing sharper conditions to entropy inequality.



## Modelling goal: Interface analysis + Numerical modelling

Two main goals to model the solid electrolyte part of the all-solid-state battery is as follows:

1. To capture the **preferred direction** behaviour of the solid electrolyte due to electric potential.
2. To satisfy **thermodynamic consistency**:
  - Conservation of mass, linear & angular momentum and energy for the solid electrolyte.
  - Entropy inequality is guaranteed with sharper conditions, which lead to constitutive equation.

$$a_{\text{Griffith}} := a^* = \arg \min_{a \in \mathbb{R}} \left( \iint_{\Omega} f(a, \mathbf{u}; \lambda, \mu, \mathbf{d} \otimes \mathbf{d}) d\Omega - \iint_{\Gamma} f(a; \gamma) d\Gamma \right) \Big|_{\mathbf{u}^{(s)}}$$

## References

- [1] T. Vo *Modeling the swelling phenomena of lithium-ion battery cells based on a numerical chemo-mechanical coupled approach*. Master thesis, 2018.
- [2] S. Braun, C. Yada and A. Latz. *Thermodynamically consistent model for Space-Charge-Layer formation in a solid electrolyte*. Journal of Physical Chem., 119, 22281-22288, 2015.
- [3] C. Hüter, S. Fu, M. Finsterbusch, E. Figgemeier, L. Wells, and R. Spatschek. *Electrode-electrolyte interface stability in solid state electrolyte sytem: influence of coating thickness under varying residual stresses*. AIMS materials Science, 4(4):867-877, 2017.
- [4] S. Kim, J. S. Kim, L. Miara, Y. Wang, S. K. Jung, S. Y. Park, Z. Song, H. King, M. Badding, J. M. Chang, V. Roev, G. Yoon, R. Kim, J. H. Kim, K. Yoon, D. Im, and K. Kang. "High-energy and durable lithium metal batteries using garnet-type solid electrolytes with tailored lithium-metal compatibility," Nature Communications, 13(1):1883, Apr 2022.

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