22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

A Unified Thermodynamic Framework: From Equilibrium and Nonequilibrium to Zentropy, Cross Phenomena, and Applications in AI and AI Safety

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Thermodynamics has traditionally been viewed as a theory of equilibrium because Gibbs formulated the combined law strictly for equilibrium systems. This historical limitation motivated the emergence of irreversible thermodynamics as a distinct field. Subsequent advances, such as Kaufman's CALPHAD modeling, Hillert's incorporation of entropy production into the combined law, and Ågren's development of atomic mobility, extended Gibbs's framework to describe materials under thermodynamic driving forces.

Building on this progression, the present author refined Hillert's nonequilibrium formalism by introducing partial internal energy, partial entropy, and partial volume directly into the first, second, and combined laws1. This refinement yields an explicit expression for the chemical potential, resolving subtle interdependencies among entropy, volume, and composition in open systems. Together with Ågren's mobility theory, it further enabled the development and later revision of the theory of cross phenomena, in which transport equations are derived from the first law and limitations of phenomenological Onsager formulations are resolved2.

In parallel, the author's team established zentropy theory3, which unifies quantum mechanics with Gibbs statistical mechanics (GSM). GSM assigns probabilities to all configurations under identical external conditions, producing a free energy landscape that represents an intrinsically nonequilibrium ensemble across stable/metastable/unstable states. Zentropy enhances GSM by providing a more accurate and hierarchical entropy framework, enabling more reliable predictions.

Together, these developments establish a unified thermodynamic framework and provide a bridge to modern AI architectures, exemplified by the zentropy-enhanced neural network (ZENN) 4. This integration yields physically grounded and interpretable predictions with internal containments that reflect both structural partitioning and zentropy-based regulation of driving forces and stability.

1 Liu, Z. K. J. Phase Equilibria Diffus. 46, 351 (2025); 2 Liu, Z. K. J. Phys. Condens. Matter 38, 015701 (2026); 3 Liu, Z. K. et al. J. Phase Equilibria Diffus. 43, 598 (2022); 4 Wang, S. et al. Proc. Natl. Acad. Sci. 123, e2511227122 (2026)