DEVELOPMENT OF RESEARCH ON SOLUTION STABILIT

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In recent years, the integration of machine learning (ML) methods with thermodynamic modeling frameworks such as CALPHAD (CALculation of PHAse Diagrams) has become a central topic in alloy design and materials science. Between November 2024 and January 2025, a series of webinars organized by Thermo-Calc Software brought together leading researchers to present advances in this area. The talks by Qing Chen [1], Ziyuan Rao [2], S. Mohadeseh Taheri-Mousavi [3], and Raymundo Arróyave [4] each highlighted different facets of ML-driven alloy discovery and optimization. These sessions showcased practical tools and case studies demonstrating how ML enhances the estimation of alloy properties and phase structures, thereby accelerating material development and improving the design of complex systems.

Together, the webinars underscore the transformative potential of integrating CALPHAD with advanced ML and AI strategies. The shift from small, limited datasets to large-scale, data-centric approaches significantly improves predictive accuracy and efficiency. Ongoing developments in generative models and Bayesian optimization are expected to further advance phase structure prediction and alloy behavior modeling.

Future research should focus on generating high-quality, physically informed data; refining multimodal ML models for greater interpretability; and combining thermodynamic simulation with autonomous experimentation. These integrated frameworks provide a promising path toward accurate and scalable estimation of alloy phase structures, contributing directly to improved stability and application of modern materials.

References:

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3. Taheri-Mousavi, S. M. *AlloyGPT: An Agent-Based LLM Framework for the Design of Additively Manufactured Structural Alloys*. Thermo-Calc Software Webinar. Available at: https://thermocalc.com/showcase/webinars/watch-alloygpt-an-agent-based-llm-framework-for-the-design-of-additively-manufactured-structural-alloys/

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