

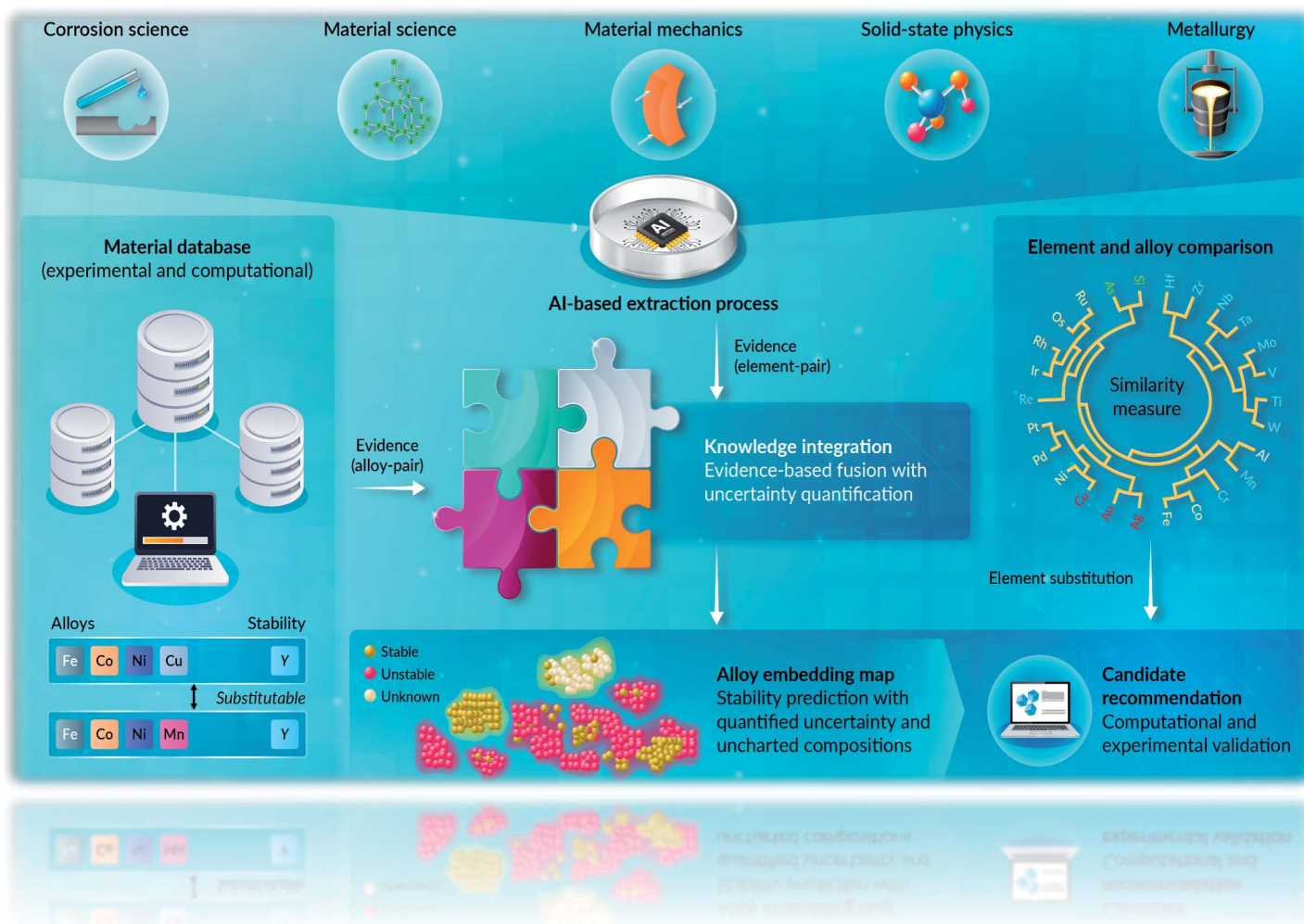
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Showing research from Professor Dam's laboratory, School of Knowledge Science, Japan Advanced Institute of Science and Technology, Ishikawa, Japan.

Beyond interpolation: integration of data and AI-extracted knowledge for high-entropy alloy discovery

This study presents an AI framework for accelerating high-entropy alloy discovery by integrating experimental data with cross-disciplinary expert knowledge. Evidence about elemental substitutions is gathered from materials datasets and from scientific literature using large language models queried in metallurgy, solid-state physics, materials mechanics, materials science, and corrosion science. These are combined using Dempster-Shafer theory to evaluate candidate alloys while quantifying prediction uncertainty. The approach achieves 86-92% accuracy even for alloys containing elements absent from training data, demonstrating how AI can fuse dispersed expert knowledge to accelerate scientific discovery.

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As featured in:



See Hieu-Chi Dam *et al.*, *Digital Discovery*, 2026, **5**, 1079.