AI-Guided Materials Design

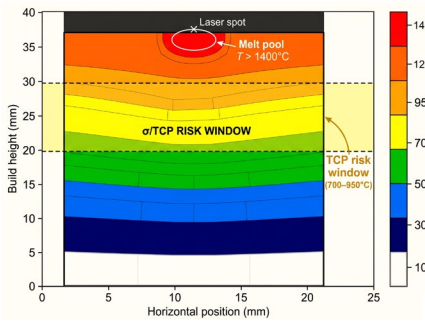
Sustainable Manufacturing and Materials Innovation

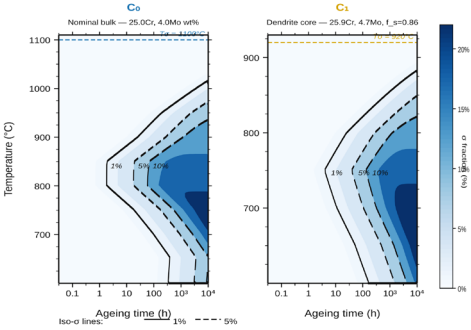
IWT
Leibniz-Institut für Werkstofforientierte Technologien

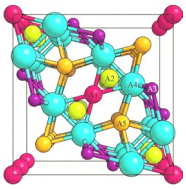
Towards accelerated materials design and manufacturing

Artificial Intelligence plays essential role in materials science and engineering. It connects numerical simulations and physical experiments into one intelligent workflow, enabling **rapid prediction, optimization and discovery of high-performance materials and processing conditions,** while reducing material and energy consumption in contrast to a trial-and-error approach.

Augmentation through AI	Key Physical Phenomena
Neuro-symbolic AI, Foundation Models	End-to-end Process-Structure-Property linkage
Bayesian Neural Networks	Residual stress, Melt pool dynamics, Thermal History
DeepONets, Fourier Neural Operators	Equilibrium, Precipitate nucleation, Dendritic solidification, Solid-state transformations
Equivariant GNNs (MACE, CHGNet)	High-throughput composition screening, Enthalpy of formation.







Simulations across the scales towards real applications (3D printing)

Funding:
Leibniz association within the project AIM (2025-2030)

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