

MONDAY

COLLOQUIUM

AI-based Hierarchical Representations of Materials for Structure–Property Prediction

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10 Nov 2025 (Monday) | 16:00 Hrs (Tea / Coffee 15:45 Hrs) | Venue: TIFRH Auditorium

Materials representation across multiple length scales is essential for enabling AI models to solve structure-to-property prediction problems in complex systems such as superalloys. Properties like Vickers hardness are primarily governed by microstructural features and formation energy correlates to atomic arrangements and, making it crucial to capture relevant information from different structural hierarchies. Accurate and interpretable representations across these scales allow machine learning approaches to accelerate materials discovery and design. At the microstructural level, three frameworks are used to represent image-based information: statistical representations using 2-point spatial correlations to capture phase distribution patterns, geometry-driven image processing techniques that extract morphological descriptors such as area, perimeter, and shape of precipitates, and deep learning models like convolutional neural networks that automatically learn hierarchical features directly from raw SEM images. These image-derived features are combined with metadata such as composition and processing history to predict mechanical properties like Vickers hardness. At the atomic level, graph-based representations like the CLEAR (Chemistry and Local Environment Adaptive Representation) descriptor-based model represents crystal structures by combining elemental properties with interatomic distances through Voronoi-based neighbours. By applying pooling operations, these graph features are transformed into fixed-size vectors that enable predictive modelling of formation energy and phase stability.