

Seminar

Accelerated materials discovery to autonomous research agents: How machine learning is transforming materials research

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I will present a broad outline of some recent developments in the application of machine learning and artificial intelligence in materials research. This will include training of ML models with available data to predict materials properties--how that accelerates materials screening, and 'inverse design' of new materials using generative AI. How these two approaches have been helped by development of machine learning force fields will also be discussed. I will briefly mention how applications of ML in analysis of experimental results have accelerated materials characterisation. I will present our work on some of these themes in this broader context. I will end by mentioning how the development of autonomous experimental agents holds the potential of radically transforming the mode of doing materials research.

Tuesday, Sep 2nd 2025

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Seminar Hall, TIFRH