Séminaire

Lundi 24 février 2025 à 14h00

Amphithéâtre Henri Benoît

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AI in Material Science

Machine learning promises to accelerate the material discovery by enabling high-throughput pre- diction of desirable macro-properties from atomic-level descriptors or structures. However, the limited data available about precise values of these properties have been a barrier, leading to predictive models with limited precision or the ability to generalise. We present a novel computational frameworks [1] suitable for predicting the physical properties of materials by performing searches over large databases. This study addresses the critical challenge posed by the limited availability of extensive datasets for thermal conductivity—a property of significant importance across applications ranging from electronics to energy storage. By using a fine-tuning method, we demonstrate our model's ability to predict the thermal conductivity of yet-to-be-synthesized compounds, with resultswithin the correct order of magnitude.

[1] https://github.com/liudakl/ParAIsite

Les personnes souhaitant rencontrer L. Klochko sont priées de prendre contact avec Olivier Benzerara.