# Optimal transfer learning strategies for property predictions in materials science

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**Abstract**

Materials science is a domain characterised by 'small' datasets (i.e., < 10,000 datapoints) of critical properties that govern performance of various applications and devices. For instance, there are no large, reliable datasets available for several key 'performance determining' metrics in energy applications, such as diffusivities in battery electrodes, carrier recombination rates in photovoltaics, and molecular adsorption energies for catalysis. On the other hand, there are reasonably 'large' datasets (> 100,000 datapoints) available on some properties, such as, bulk formation enthalpies, computed band structures, and crystal structures across wide chemical spaces. Thus, if key chemical, compositional, and structural trends can be captured in available large datasets and subsequently transferred (or re-learnt), it will enable the use of deep learning and graph based neural network models in smaller datasets as well. Hence, my talk will explore the utility of current transfer learning (TL) approaches that are available for computational materials science and identify optimal ways to employ TL-based strategies. Specifically, TL involves training a neural network model on a larger dataset and subsequently retraining a fraction of the model on a smaller dataset. I will quantify the accuracy, transferability, and efficiency of TL models compared to models that have been trained from scratch. Finally, I will focus on TL models that can generalise over multi-properties during pre-training and can efficiently be re-trained on small datasets, which pave the way towards creating more general, foundational models, in the near future.

Keywords: Transfer learning, Materials Properties, Multi-property training

**Description of work**

In the realm of materials design and optimization, machine learning (ML) architectures have played a pivotal role given their ability to predict material properties at low computational costs. However, there are several materials properties that critically govern the efficiencies of devices which are notoriously hard to predict (and train) ML models. For example, ionic conductivity in electrolytes employed in batteries, defect formation energies of semiconductors, and surface properties of key materials used in catalytic applications. The primary limitation in training of reliable ML models on such critical material properties is the lack of availability of 'large' datasets (i.e., > 100,000 datapoints), with currently available experimental and/or computational datasets often being 'small' (< 10,000 datapoints). Given that training of reliable deep learning (DL) models require large datasets, an alternative strategy is required to predict such material properties quickly.

Importantly, transfer learning (TL) is a promising strategy to train DL models with sparse datasets, which has been demonstrated in computer vision and in biological applications. Briefly, TL involves a DL model that is pre-trained (PT) on a larger, easily-available dataset (e.g., formation energies of materials) and subsequently fine-tuned (FT) on the target datasets that are often small (e.g., piezoelectric modulus). Thus, we identify the optimal strategies [1] to perform TL among various materials datasets using the atomistic line graph neural network (ALIGNN) architecture. Specifically, we optimize the model architecture, tune the hyperparameters, identify optimal ways to sample sparse datasets, and observe the amount of retraining required during FT for good performance. Additionally, we demonstrate the utility of the TL approach in swiftly predicting materials properties, especially against models trained from scratch. Also, we show that TL models generally learn properties (upon FT) much faster (i.e., at fewer datapoints) compared to scratch models.

In addition to identifying optimal TL strategies, we also demonstrate a pathway to create models that are generalizable over a wide range of materials properties. Specifically, we train ALIGNN models simultaneously over multiple material property datasets, by modifying the prediction head, resulting in models that are PT on multiple properties (or MPT models). Subsequently, we demonstrate that the MPT models perform better than both scratch and PT-FT models on 4/6 occasions. Moreover, we show that the MPT models generalize significantly better on an out-of-domain dataset consisting of properties of two dimensional materials, which is fully different from the three dimensional bulk properties used during PT. Thus, we demonstrate an architecture that can be used to generalize across multiple properties efficiently and can be systematically made better by including more properties during PT in the near future.

We hope that our work enables the creation of reliable TL and generalizable models, further accelerating property predictions among materials, resulting in materials discovery for novel applications.

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## References

[1] https://arxiv.org/abs/2406.13142