

## Machine Learning for Heusler Alloys in Spintronic Devices

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Heusler alloys have long been proposed as the building blocks of spintronic devices due to the possibility to "select" their properties based on their composing elements, ordering, etc. These properties give rise to spintronic effects that are the core of a prospective device: high spin polarization, high anomalous Hall angle, topological insulating behaviour, amongst others.

Although the properties of a myriad of full and half Heusler alloy compositions have been predicted from first principles and corroborated experimentally, no path was clear to produce devices using these materials. This is mainly due to the complexities of growing them in thin films in addition to the use of deposition techniques and high processing temperatures that are not compatible with the current industrial processes. Yet, in the last couple of years, the ambient or room temperature sputtering of device-relevant Heusler alloys was demonstrated, opening the door for these materials to be integrated into potential devices. With this, a new challenge arises: finding Heusler alloys with strong spintronic effects at reduced dimensions and relevant operation conditions.

When searching for new materials, it is useful to enlist the help of computational materials science: that is, using computer simulations to test the properties of a material before subjecting it to testing in the laboratory. This pre-screening tends to require far fewer resources in terms of cost and time. However, some problems remain: namely, the quantum-mechanical calculations needed still require a significant amount of time and are often limited to looking at small representative structures. It is here that modern machine-learning methods, which allow the accurate prediction of quantum-mechanical properties for more complex systems, come into play.

In this project, you will:

- Perform quantum-mechanical calculations to populate the Heusler alloy database
- Develop and train machine learning models for property prediction, Initially aimed at maximizing the anomalous Hall effect coefficients of bulk and thin-film alloys
- Execute high-throughput structure searches for optimal candidates
- Collaborate with experimentalists in the School of Maths and Physics for synthesis and validation

Key transferable skills developed:

- Critical Thinking
- Machine learning
- Collaboration with academia and industry

Funding:

This project is part of the Enhanced Postgraduate Skills Doctoral Training Programme (EPS DTP [Enhanced Postgraduate Skills - Doctoral Training Programme | About | Queen's University Belfast](#)). This programme offers an enhanced stipend of an additional £5000 per year, a Research Training support budget of £5000 per year, industry mentoring, 3.5 years in duration, CMI Level 7 training.

This project is open to Home studentships only - cover tuition fees and include a maintenance stipend of £21,805 per annum.

An industry gross salary (pre-tax, student loan repayment, pension (3%) and national insurance contributions) of over £33,000 results in an approximately equivalent take home pay.

A Home studentship is open to UK and ROI nationals, and to EU nationals with settled status in the UK, subject to meeting specific nationality and residency criteria.

DfE studentship eligibility information can be viewed at: <https://www.economy-ni.gov.uk/publications/student-finance-postgraduate-studentships-terms-and-conditions>

Annual stipend top-up of £5,000 also included.