

PO-YEN TUNG

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Machine Learning Projects

Alloy Discovery

Active learning workflow for high-entropy alloy design

- Combined **generative model** with **physics-driven simulation** and **experiments**
- Discovered **2 optimal alloys** out of millions of possible compositions in **3 months**
- Published in [Science](#)

Derivative-free optimisation for complex systems

Black-box optimisation for fast and optimal design of complex systems

- Outperformed **all** state-of-the-art methods ([paper](#))
- Employed dynamic **upper confidence bound** and **back-propagation** with neural network
- Showed effectiveness for **real-world** problems (e.g. cyclic peptide binder and architecture design)

Self-supervised Chemical Spectrum Analysis

Open-source tool [SIGMA](#) to automate the chemical analysis of electron microscopic data

- Capable of carrying out **anomaly detection** for unique chemical signals
- Conducted with **autoencoder** and **Gaussian mixture model** in Python and PyTorch
- Outperformed the state-of-the-art algorithm by 30% accuracy

Object Detection for 2D Electron Diffraction Analysis

Novel object detection algorithm to solve 2D electron diffraction orientation solutions

- **Surpassed all existing methods** in performance and slashed the computation time by 50%
- Uncovered a new connection between the detection model and crystallographic principles
- Implemented in Pytorch, PyTorch-Lightning and Hydra

Skills

Language : Python, Java

Technologies : PyTorch, PyTorch-Lightning, Tensorflow, Hydra, Numpy, Pandas, Scikit-learn

Machine Learning: Self-supervised learning, Generative models, Transformer, Computer vision

Professional Experience

University of Cambridge

Cambridge, UK

Research Associate in Machine Learning - Department of Materials Science Sep 2021 – Present

- Creating and applying cutting-edge machine-learning methods for electron microscopy

Education

Max Planck Institute

Düsseldorf, Germany

PhD in Materials Science

Mar 2018 - Jul 2021

- *Subject area:* **machine learning** for materials discovery, **machine learning** for material characterisation
- *Courses:* linear algebra, statistics, statistical machine learning, machine learning