Using Generative Adversarial Networks to match experimental and simulated inelastic neutron scattering data

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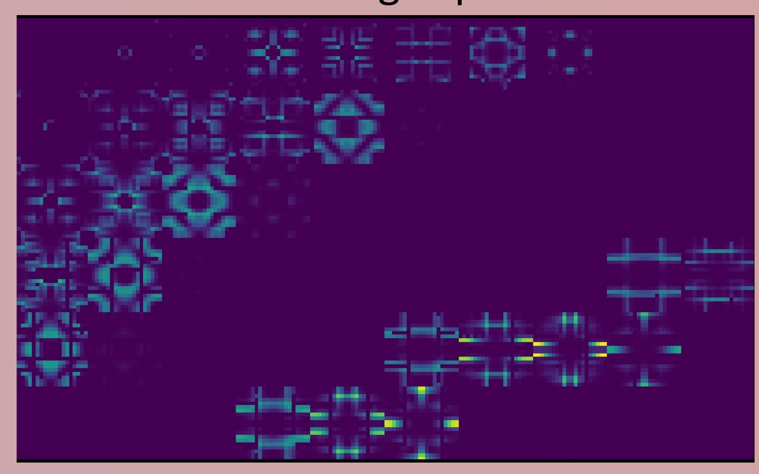
Introduction

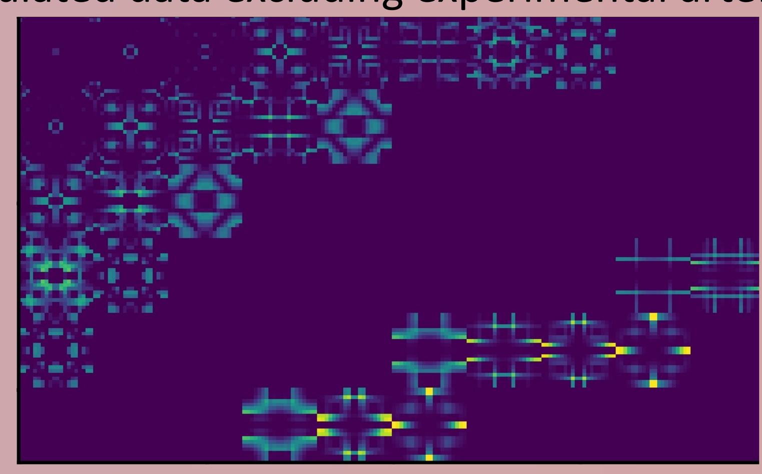
During the past decades, research in materials science has been accelerated by the rapid development of synchrotron and neutron sources.[1] Conventional data analysis approaches using minimization techniques, such as least-squares fitting algorithms, cannot keep up with the increasing size of measured datasets. Consequently, data analysis is becoming a bottleneck for research in materials science.[2-3] Therefore, it is of great importance to improve the current state-of-the-art for data analysis for materials science, particularly utilizing recent developments in artificial intelligence and machine learning (ML).[2-4] One of the unsolved problems in this context is to match the simulated datasets that the ML algorithms are trained on to the experimental datasets. This has particularly been a problem for the analysis of inelastic neutron scattering (INS), where it is computationally expensive to ensure that simulated data correctly mimics the experimental signal and background.[5]

[1] Wang, C. et al., *Synchrotron Big Data Science,* Small **2018**. [2] Agrawal, A. et al., *Perspective: Materials informatics and big data: Realization of the "fourth paradigm" of science in materials science,* APL Materials **2016**. [3] Butler, K. T. et al., *Machine learning for molecular and materials science,* Nature **2018**
[4] Hey, T. et al, *Machine learning and big scientific data*, Phil. Trans. R. Soc. Lond. A **2020**. [5] Butler, K. T. et al., *Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data* , J. Phys.: Condens. Matter **2021.** [6] https://spinw.org/

Simulated data including experimental artefacts



Simulated data excluding experimental artefacts

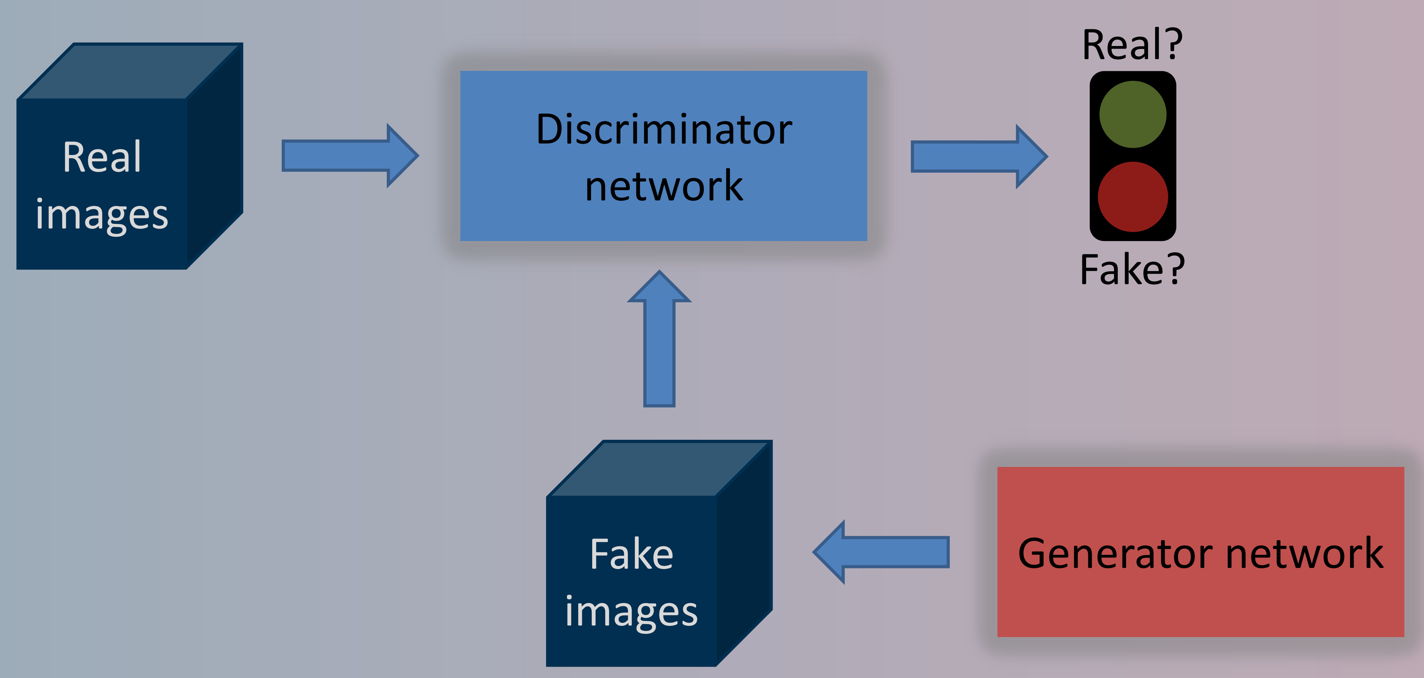


The concept of a generative adversarial network (GAN)

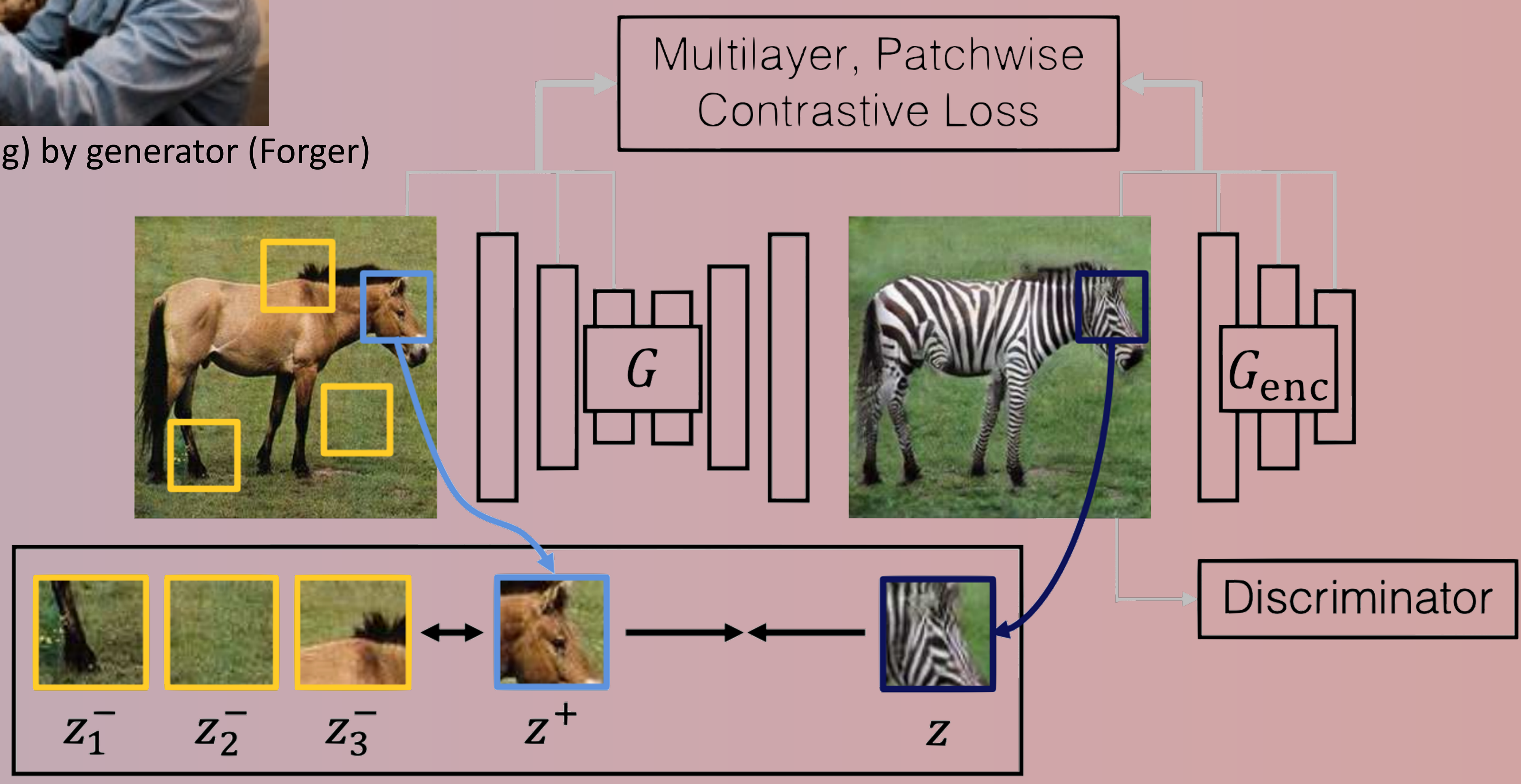
Real data (Paintings)

Fake data (painting) by generator (Forger)

General architecture of a GAN



Our GAN architecture



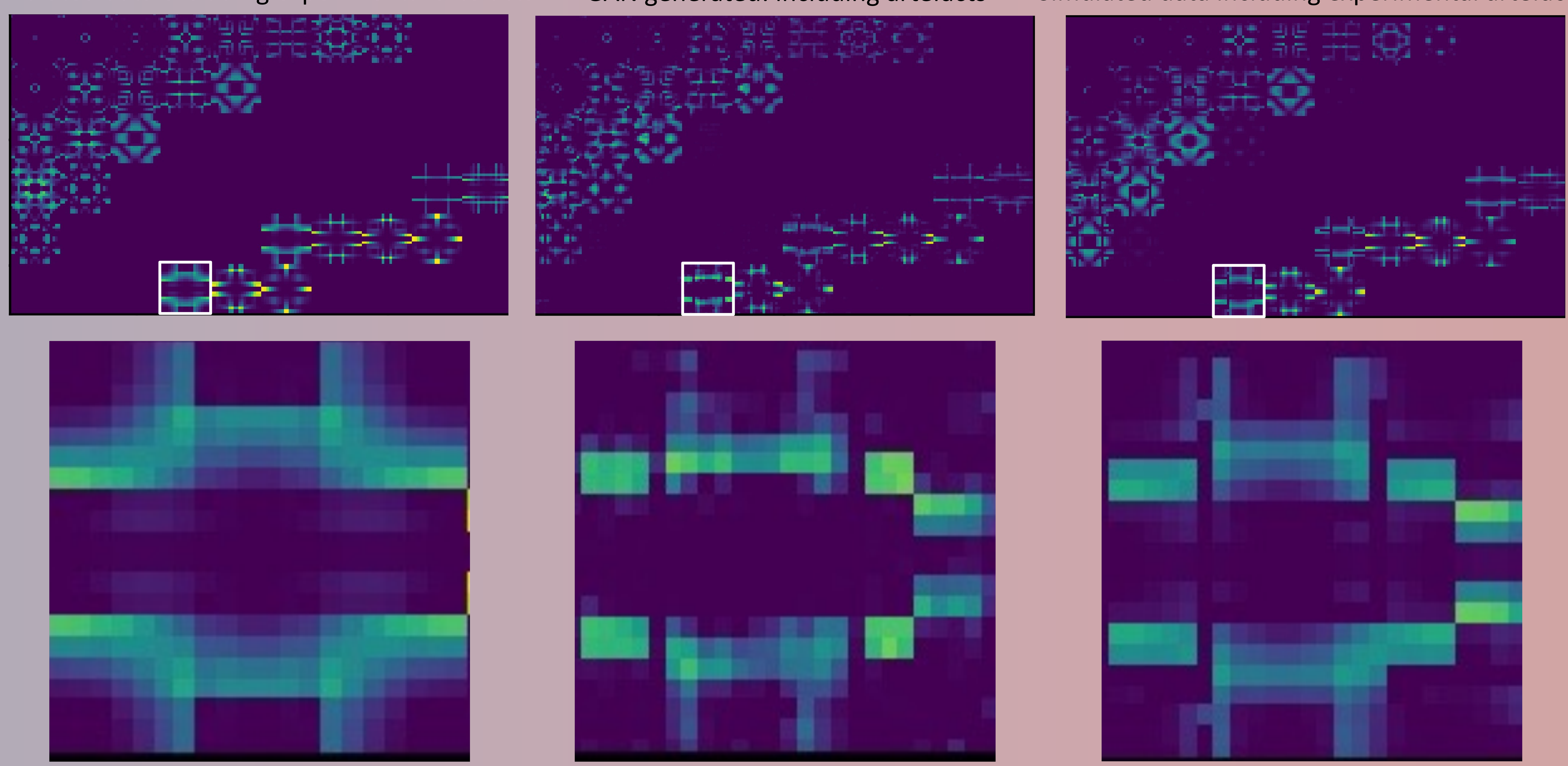
Patchwise Contrastive Learning

Park, T., et al., *Contrastive Learning for Unpaired Image-to-Image Translation, ArXiv **2020***

Matching experimental and simulated inelastic neutron scattering (INS) data

We are developing generative adversarial networks (GANs) that can learn to make simulated INS data that matches experimental INS dataset under a second. This GAN-based approach, once trained, will be deployed in a range of scenarios for analysing and understanding INS dataset. The GAN can be used to help classify materials structures from the INS datasets and to work with other ML and non-ML (e.g. Spin-W[6]) algorithms which can estimate magnetic Hamiltonian parameters from INS data.

Simulated data excluding experimental artefacts | GAN generated: including artefacts | Simulated data including experimental artefacts



Acknowledgments

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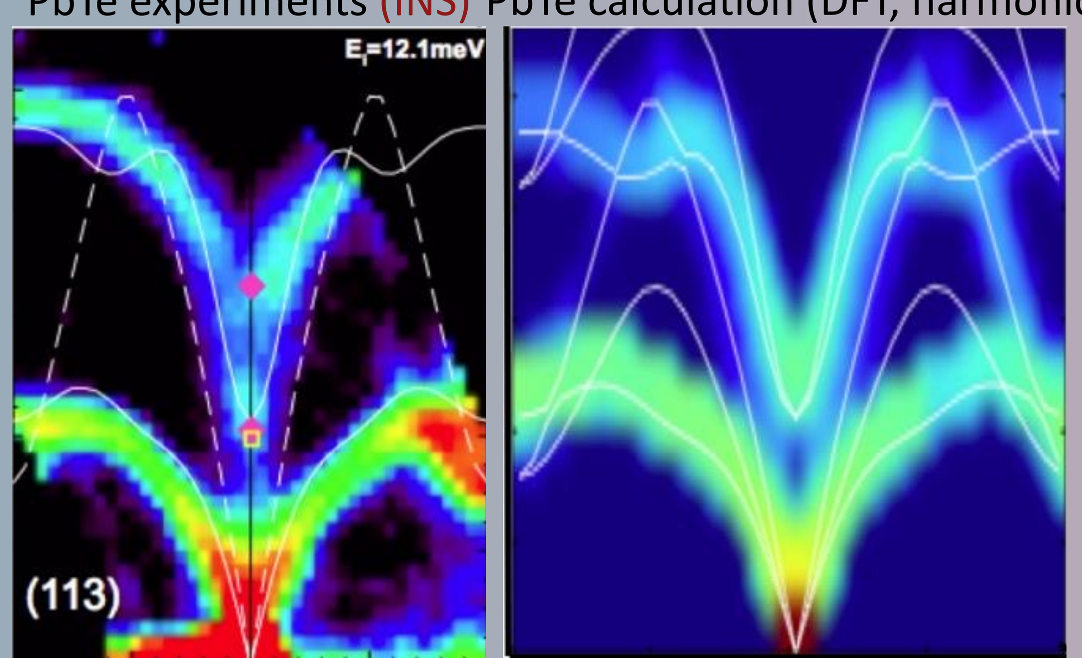
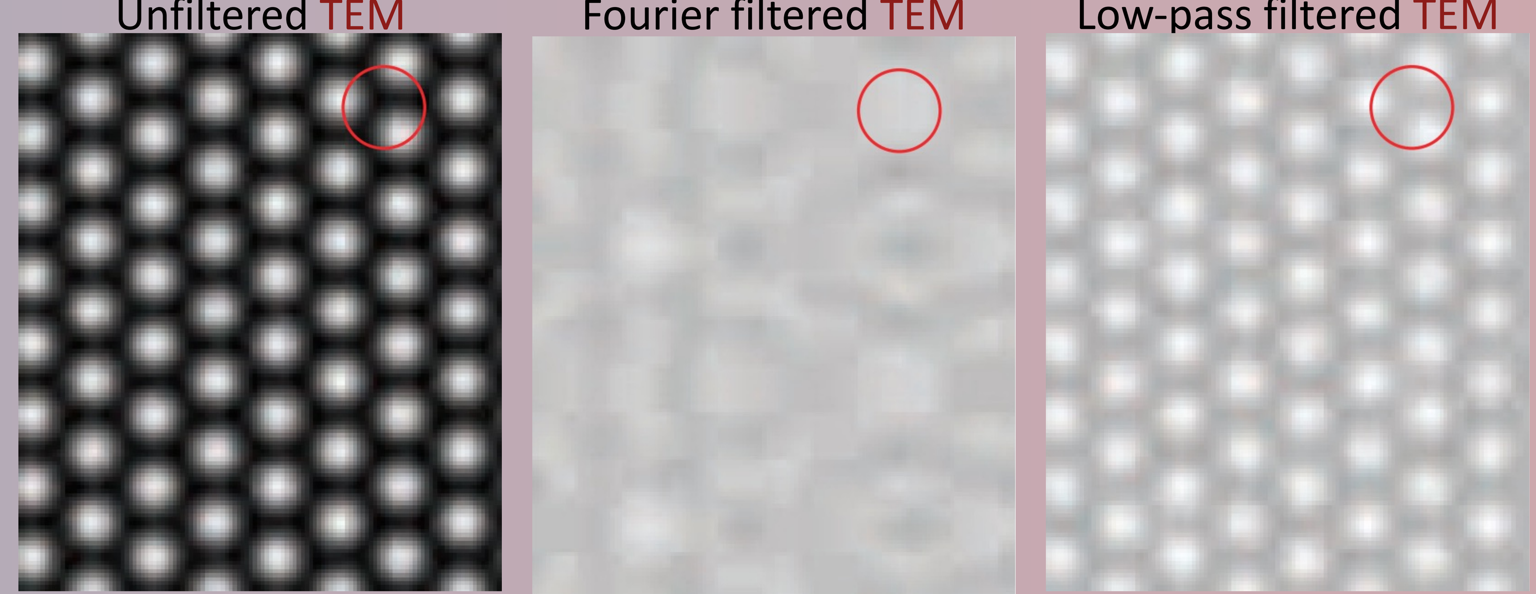
The aim is to expand the GAN to match simulated and experimental datasets for a range of techniques

PbTe experiments (INS) PbTe calculation (DFT, harmonic)



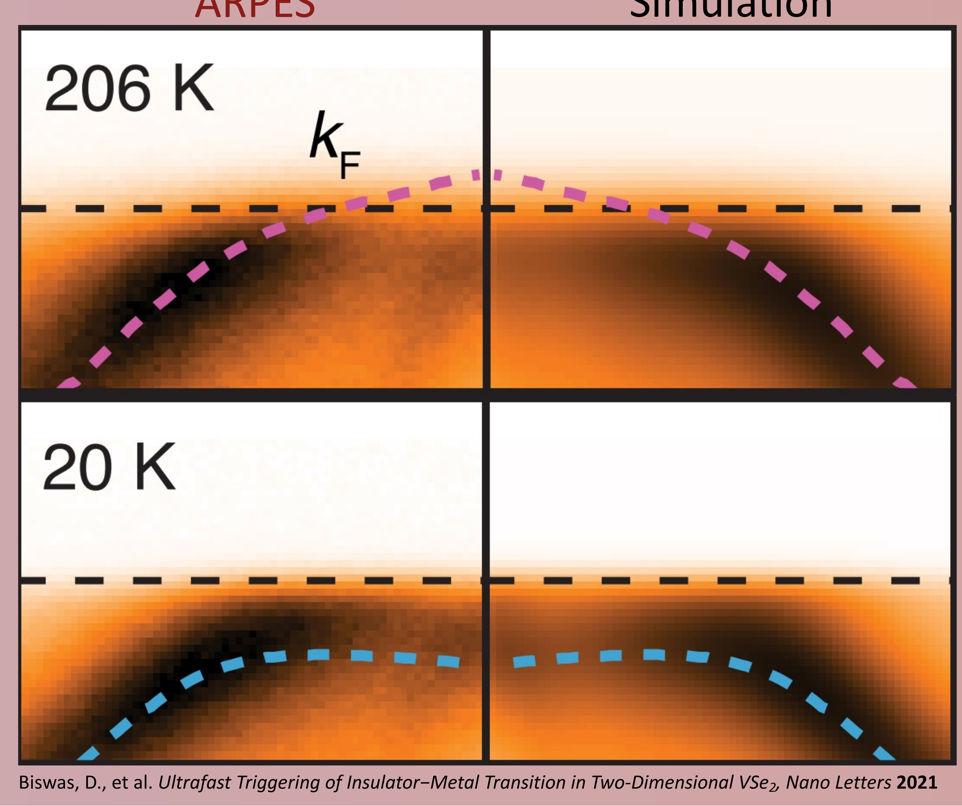
Delaire, O., et al. *Giant anharmonic phonon scattering in PbTe, Nature Materials* **2011**

Unfiltered TEM | Fourier filtered TEM | Low-pass filtered TEM



Meyer, J. C., et al. *Experimental analysis of charge redistribution due to chemical bonding by high-resolution transmission electron microscopy, Nature Materials* **2011**

ARPES | Simulation



Biswas, D., et al. *Ultrafast Triggering of Insulator−Metal Transition in Two-Dimensional VSe_2, Nano Letters* **2021**