

# Machine Learning from the Large Hadron Collider to van der Waals Materials

**Sonia Conesa-Boj**<sup>1</sup>, Abel Brokkelkamp<sup>1</sup>, S. van der Lippe, Isabel Postmes<sup>1</sup>, Laurien I. Roest<sup>1</sup>, Sabrya E. van Heijst<sup>1</sup>, Juan Rojo<sup>2</sup>

<sup>1</sup>Kavli Institute of Nanoscience, Delft University of Technology, 2628CJ Delft, The Netherlands

<sup>2</sup>Nikhef Theory Group, 1098 XG Amsterdam, The Netherlands; Physics and Astronomy, Vrije Universiteit Amsterdam, 1081 HV Amsterdam, The Netherlands

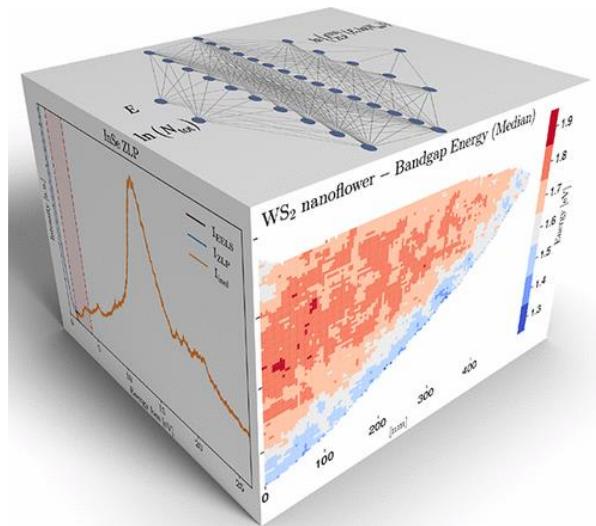
s.conesaboj@tudelft.nl

Machine learning (ML) methods have witnessed an impressive progress in the recent years in tasks such as automated signal identification, pattern recognition and classification, anomaly detection, uncertainty quantification, and unbiased background removal. In this talk, I present applications of ML in data processing for Scanning Transmission Electron Microscopy (STEM) analyses of van der Waals materials, using algorithms inspired by use cases in high-energy physics. These approaches are essential to fully exploit the high-quality multi-dimensional datasets provided by state-of-the-art detectors. The manual processing and interpretation of these high-dimensional datasets is however time-consuming and error-prone, and ML methods offer a powerful toolbox to automate and streamline the full analysis pipeline. First, we demonstrate how ML efficiently removes large background contributions in the low-loss region of Electron Energy-Loss Spectroscopy (EELS), enabling the identification of bandgap energy modulations [1,2]. Second, the combination of unsupervised learning with four-dimensional (4D) STEM enables the precise characterization of nanoscale strain fields across micron-sized specimens [3,4]. Third, automated feature identification in low-loss EELS measurements makes possible the detection of exciton confinement in one-dimensional MoS<sub>2</sub> nanostructures [5]. Finally, I outline potential future applications of ML in TEM data analysis, including enhanced mapping of local polarization and automated feature identification in EELS spectra.

## References

- [1] L. I. Roest, S. E. van Heijst, L. Maduro, J. Rojo, and S. Conesa-Boj, Ultramicroscopy, 222 (2021) 113202.
- [2] A. Brokkelkamp, J. ter Hoeve, I. Postmes, S. E. van Heijst, L. Maduro, A. V. Davydov, S. Krylyuk, J. Rojo, and S. Conesa-Boj, J. Phys. Chem. A, A126 (2022) 1255.
- [3] M. Bolhuis, S. E. van Heijst, J. J. M. Sangers, S. Conesa-Boj, Small Science, 4 (2024) 2300249.
- [4] S. E. van Heijst, M. Bolhuis, A. Brokkelkamp, J. J. M. Sangers, S. Conesa-Boj, Advanced Functional Materials, 34 (2024) 2307893.
- [5] S. van der Lippe, A. Brokkelkamp, J. Rojo, S. Conesa-Boj, Advanced Functional Materials, 33 (2024) 2307610.

## Figures



**Figure 1.** Schematic illustration showing how high-dimensional measurements from Scanning Transmission Electron Microscopy can be efficiently processed using machine learning techniques inspired from particle physics.

