ADVANCES IN MACHINE LEARNING METHODS FOR THE DETERMINATION OF ELECTRON SCATTERING CROSS-SECTION SETS

D. L. MUCCIGNAT¹, G J BOYLE¹, N. A. GARLAND² and R. D. WHITE¹

 1 College of Science and Engineering, James Cook University, Townsville 4810, Australia E–mail dale.muccignat@my.jcu.edu.au

² Centre for Quantum Dynamics, Griffith University, Nathan 4111, Australia \mathcal{C} School of Environment and Science, Griffith University, Nathan 4111, Australia

Abstract. Accurate modelling of electron scattering from complex biological targets is critical for the development and implementation of plasma devices in fields such as medicine, nanoscale device manufacturing and agriculture [Adamovich et al.]. Underpinning these models are complete and self-consistent electron scattering cross-section sets that provide a microscopic description of electron scattering for a particular target molecule. While there exists a wealth of cross section set data available for select molecular targets in databases such as LXCat (see www.lxcat.net), the same can not be said for an ever growing number of molecular targets that are important for industrial and scientific applications.

A key focus of the research group at James Cook University has been to develop new, and improve existing, numerical techniques to assist in the determination of complete and selfconsistent electron scattering cross-sections sets from experimental data. In particular, we focus on using deep learning methods to solve of the ill-posed 'inverse swarm problem', which aims to derive cross-section data from experimentally measured swarm transport coefficients.

We first present a brief history of the inverse swarm problem and outline the ill-posed nature of its solutions. We then present an overview of existing deep learning methods before highlighting the improvements made in a recent publication [Muccignat *et al.*]. We then present a preliminary investigation into the application of mixture density networks to determine the uncertainty of deep learning solutions to the inverse swarm problem. Finally, we conclude by summarising the existing limitations of deep learning methods and highlight the experimental and numerical data needed for future investigations.

References

Adamovich, I. et al. : 2017, J. Phys. D: Appl. Phys., **50**, 323001 Muccignat, D. L. et al. : 2024, Machine Learning: Science and Technology, **5**, 015047