



## PHD PROJECT DESCRIPTION

<b>Project Title:</b> * Rapid screening of surface reaction networks using physics-informed machine learning
<b>Supervisor(s) Name and E-Mail(s):</b> *
Dr Sherif Abbas <a href="mailto:s.abbas@deakin.edu.au">s.abbas@deakin.edu.au</a> Prof Truyen Tran <a href="mailto:truyen.tran@deakin.edu.au">truyen.tran@deakin.edu.au</a>
<b>Project Description:</b> *
<p>Predicting the fate of a chemical reaction is highly complex and is one of the key challenges in chemistry. It requires the computation of a large number of possible reaction products that might result from a large number of possible reaction pathways; a network of reaction pathways connecting reaction products. To find the most probable reaction pathways, and hence reaction products, the nodes of this massive network (reaction products) must be computed using highly accurate, as well as expensive, first principal quantum chemistry methods. The complexity of these reactions increases when the size of the molecules increases in the gas phase. The problem becomes even more complex when the reactions happen on a surface: on the surface, the cost of first principal quantum chemistry becomes much higher than in the gas phase.</p> <p><b>Challenge and aim</b></p> <p>This project aims to invent machine learning methods that can enable the efficient enumeration and computation of the reaction networks on surfaces. To this end, the project will develop novel machine learning representations and models to perform molecular dynamics at the scale of tens of nanometres. The candidate is expected to invent new physics-informed machine learning methods and tools to enhance the accuracy and efficiency of the computations. The success of this project will have far reaching impact on the science and practice of surface chemistry, such as in corrosion science, catalysis and retrochemistry. In corrosion science, the project can inspire new coating materials that can act as corrosion inhibitors, and can unravel new insights on the corrosion mechanisms that cannot be obtained by state-of-the-art first principles simulations. In catalysis, the project can inspire new methods for fine tuning the composition and structure of heterogeneous catalysis. In retro chemistry, the efficient generation of reaction networks can enable the exploration of synthesis pathways that involve surface catalysts.</p>
<b>Preferred special skills and expertise:</b> * e.g., qualification, publications, registrations, memberships (if applicable)
<ul style="list-style-type: none"><li>• Postgraduate degree in computer science, physics, chemistry or mathematics</li><li>• Publication of at least 1 article in a peer-reviewed journal on AI fundamentals, AI applications or chemistry</li></ul>