## School of Chemistry:

| | |
|---|---|
| **Academic Researcher:** | **Associate Professor Ivan Kassal** |
| **Project Title:** | **Advanced organic electronics** |
| **Project Summary:** | This project aims to identify design rules for next-generation organic electronics, especially organic solar cells. It will use both computational simulations and experimental work to understand and improve organic electronic devices. |
| **Project Synopsis:** | How organic solar cells convert light into electricity is still not completely understood. The most perplexing aspect is why the positive and negative electric charges drift apart despite being strongly attracted to each other. This project will develop new simulation tools to better understand these fundamental processes, and then test them experimentally. The theory component will involve multiscale modelling to bridge the vastly different length scales that are important in organic electronics, all the way from atoms to full devices. Doing so will involve combining methods such as kinetic Monte Carlo with macroscopic drift diffusion models. The theoretical results will then be tested experimentally to confirm the predictions or provide data to refine them. The project can be tailored for the successful candidate to range from a focus on theoretical modelling of multi-scale processes to a mix of theory and experimental device study. |
| **Additional Information:** | Applicants should have a strong background in physical chemistry, chemical physics, or materials science, in either theory or experiment (or both). |

| | |
|---|---|
| **Academic Researcher:** | **Dr Asaph Widmer-Cooper** |
| **Project Title:** | **Using computer simulations to design better printable solar cells** |
| **Project Summary:** | The ability to print efficient, stable and cheap solar cells near ambient conditions would revolutionise our transition to renewable energy.<br>Metal halide perovskites have emerged as a promising candidate for realising this dream, as a printable solar cell material with the fastest growing efficiency to date.<br><br>The ARC Centre of Excellence in Exciton Science, in partnership with CSIRO, is working to make this a reality by combining a multidisciplinary research team with pilot-scale printing capabilities.<br>In this project, you will use computer simulations to study how crystalline films of metal halide perovskites form from solution and how they are affected by moisture. The insights gained from this work will help our experimental partners to obtain better control of device nanostructure and performance.<br><br>The Centre of Excellence in Exciton Science is funded by the Australian Research Council and links the University of Sydney, the University of Melbourne, Monash University, RMIT and UNSW, together with other national and international partners.<br>As a PhD student in the Centre, you will be part of a network of over 100 students and scientists, with regular opportunities to take part in scientific meetings and training programs. For further information about the Centre. This project will include the opportunity to visit experimental collaborators in Melbourne. |
| **Project Synopsis:** | Metal halide perovskites are inorganic or organometallic materials that can be formed into thin crystalline films by depositing a solution of precursor ions onto a substrate and then removing the solvent. This process has been used to make very efficient perovskite solar cells (PSCs) at small scale, however there are |

| | |
|---|---|
| | barriers to converting this success into a mature technology. For example, PSCs are not as stable under humid environmental conditions as conventional silicon-based solar cells, and it is not currently possible to print efficient PSCs at scale.<br><br>One of the central problems is that we lack a detailed understanding of how perovskite crystals form at the molecular level and of how to influence this process. To help solve this problem, you will use computational modelling to study the formation and dissolution of metal halide perovskites at the molecular level. This will involve the use of molecular dynamics simulations and statistical mechanics techniques to characterise the mechanism and thermodynamics of these processes, including the effect of changing experimental conditions. This will be done in close collaboration with experimental partners in Melbourne and with other members of our diverse research group at the University of Sydney.<br><br>The expected outcome is a set of strategies (ink formulation and processing conditions) that can be used to print stable and efficient PSCs at scale. |