# Pioneering the combinatorial method for designed plasmonic materials applied to clean energy

**Dr Tristan Temple, Macquarie University, 2015**

The project aim was to employ combinatorial materials science approach to produce novel advanced materials which will make solar energy conversion more efficient.

We focussed in the use of **metallic nanostructures to** improve the capture of light energy. These behave like optical antennas and concentrate light into the active regions of the material. The antenna properties of metallic nanostructures arise from the excitation of localized surface plasmons, electric charge oscillations excited by light. **We took advantage of combinatorial materials science which provides a paradigm for speeding up the discovery process** by enabling rapid optimizing of the material and structure parameters. By using advanced deposition systems at CSIRO Lindfield site (S. Dligach) we have been able to understand the role optical properties play in the optimised solar cell reflectors, and carefully optimise the spacer layers that control the performance of antireflection coatings critical for solar cells. Both results have been published in refereed journals. Other aspects of this project have been presented at several national and international conferences as listed below. Specific technical achievements included:

- Using a combinatorial design approach to optimise the size and position of metal nanoparticles for antireflection (AR). Samples included gold and silver nanoparticles with sizes ranging from 5nm to 300nm, and a spacer layer ranging from 0nm to 100nm. An optimum spacer thickness of 50nm for all particle sizes demonstrated a reduction of integrated reflectance from 46% to 9% across the 300-1000nm spectral range.

- A gradient deposition process has been developed and optimised, enabling the fabrication of samples with graded thickness along either 7.5cm or 15cm sample lengths. This enabled the rapid fabrication of samples covering an extremely wide parameter space, and is the backbone of our combinatorial approach. Modifying the mask design allowed us to finely tune the gradient parameters.

- An aluminium nanoparticle (Al NP) fabrication technique has been developed, with in-situ ellipsometry providing extremely high fidelity control over the growth process. Al NPs show great promise for solar cells because Al is considerably more abundant and lower cost than Ag or Au.

- We have demonstrated that ion-beam milling (IBM) can be used to modify the three- dimensional shape of metal nanoparticles. This provides an additional degree of freedom in the design of nanoparticles, without increasing the complexity or the throughput of the fabrication technique. For example a 15min Ar ion bombardment (200V, 2A) shifts the resonance of ~50nm Au NPs from 585nm to 697nm. Using IBM to reduce the height of metal nanoparticles also greatly decreased the overall surface roughness of the array, which is essential for the subsequent growth of high quality semiconductor layers for solar cells.

- We have continued to improve the accuracy of simulations by studying the influence of optical constants and also the influence of ultrathin contamination layers on metal nanoparticles. Contamination layers may form due to exposure to air or due to the use of chemical treatment, and we have identified the range of material parameters that should be maintained to ensure the nanoparticles exhibit strong resonances and low loss. Specifically, nanoparticles with diameter larger than 95nm yiled less than a 2% degradation of optical cross-section provided the extinction coefficient of the contamination shell is less than 0.1.

- The parameter space for plasmonic enhancement of solar cells is exceptionally large, and thus far only a small fraction has been explored in the literature. We have established robust methods to considerably expand this search with minimum complexity, and using an industrially relevant fabrication technique. We have shown that combinatorial optimisation is required to produce metal nanoparticle arrays that outperform conventional antireflection coatings.

The appointed Fellow Dr Tristan Temple has been encouraged to broadly engage with the research community and to build his career and research links. During his Fellowship he visited key overseas laboratories at the Technical University of Delft, Netherlands, and at Southampton University, UK as well as AIST in Japan with whom he developed a research partnership. He also established contacts with the CSIRO Energy Technology division at Newcastle, Australia. To establish my reputation in the Australian plasmonics and photovoltaics communities he visited groups at UNSW, Melbourne, Monash, Swinburne Universities, UTS, ANU where he also gave presentations. He also gave presentations at CSIRO Lindfield, at Macquarie University and hosted research visitors. He independently supervised 2 overseas students on 6 months project where he significantly contributed to project planning and its oversight. He gave a significant number of guest lectures (over 12) in the undergraduate Physics program at Macquarie and made strong contributions to Macquarie science outreach activities (Scientists in Schools, Robotic Challenge). He undertook technical training workshops and seminars in the use of ellipsometry, Comsol Multiphysics, photoresist processing and focused ion beam including a specialised workshop in Adelaide. He enhanced his funding track record with applications to JSPS Open Partnership Joint Projects and for the Australian Nanotechnology Network Overseas Travel Fellowship.