



## <sup>3rd</sup> MANA & GREEN The 73<sup>rd</sup> The 10<sup>th</sup> Joint Seminar



Beyond Perovskites: Chemical Principles for Next-Generation Solar Energy Materials Chair: Dr. Yoshitaka TATEYAMA (MANA PI / Group Leader of IFCS-Gr., GREEN)

## Prof. Aron Walsh

(Imperial College London, UK)

Theory and simulation is becoming an increasingly powerful tool in materials science. Developments in artificial intelligence have the potential to supercharge the materials discovery process. I will discuss the role that predictive modelling can play in the design of photovoltaics from the high-throughput screening of candidate compounds, the rigorous assessment of physical responses, to the optimisation of device architectures. Particular attention will be paid to what can learned from the high-performance of perovskite solar cells. Examples will be taken from our exploration of kesterite (e.g. Cu2ZnSnS4), matlockite (PbFCl type), herzenbergite (SnS), and antimonselite (Sb2Se3) systems.

## Venue: Auditorium, 1F, WPI-MANA Bldg., Namiki-siteDate: June 10th, MondayTime: 15:00-16:00

Contact: International Center for Materials Nanoarchitectonics (MANA)