# DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
# VIRTUAL SEMINAR SERIES
# FALL 2020

**DATE:** WEDNESDAY, NOVEMBER 18

**TIME:** 1:00-2:20pm

**LOCATION:** Meeting number: 120 119 5689
Password: EuWfUyEJr0YsiA
https://njit.webex.com/njit/j.php?MTID=me5749cc7a258e4d25900ac3478371cb7
**Join by video system**
Dial 1201195689@njit.webex.com
You can also dial 173.243.2.68 and enter your meeting number.
**Join by phone**
1-650-479-3207 Call-in toll number (US/Canada)
Access code: 120 119 5689

## GUEST SPEAKER

Professor Aron Walsh
Department of Materials
Imperial College London, UK

## TOPIC

Computer-Accelerated Materials Design

## ABSTRACT

The theory and simulation of molecules and materials has become increasingly accurate and predictive over the past few decades. The process of computing the chemical and physical properties of a known compound is now well established. The next challenge is to explore the vast space of unknown compounds, and to identify materials with the properties required to support the next-generation of technologies. This is being supported by rapid developments in both hardware (classical supercomputers and the first commercial quantum computers) and software (new algorithms and statistical approaches). Transfer of knowledge from the artificial intelligence community has the potential to supercharge chemical discovery by accessing a large phase space of potential compounds that is inaccessible by high throughput experiments or traditional calculations alone [1,2]. After providing a snapshot of the current status and future direction in this field, I will illustrate developments from our recent progress in the description of materials used in solar energy technologies [3,4]. Current bottlenecks in the field, including the absence of reliable and comprehensive structure-property databases, will be discussed.

[1] “Computational screening of all stoichiometric inorganic materials” Chem 1, 617 (2016) [link]
[2] “Machine learning for molecular and materials science” Nature 559, 547 (2018) [link]
[3] “Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites” Nature 580, 360 (2020) [link]
[4] “Upper limit to the photovoltaic efficiency of imperfect crystals” Energy and Environmental Science 13, 1481 (2020) [link]

## BIO

Aron Walsh is Professor of Materials Design at Imperial College London, UK. He holds a dual appointment as an Underwood Distinguished Professor at Yonsei University, Korea. Aron was awarded his PhD in Chemistry from Trinity College Dublin and completed a postdoctoral position at the National Renewable Energy Laboratory (USA). He began his independent research career at the University of Bath and held a Royal Society University Research Fellowship in the Department of Chemistry. His research combines technique development and applications at the interface between solid-state chemistry and physics. He has over 350 publications, which have gathered over 35,000 citations, placing him on the Clarivate Highly Cited Researchers List. In 2019, Aron was awarded the Corday-Morgan Prize from the Royal Society of Chemistry and became a Scientific Editor of their flagship journal Materials Horizons.

**Committee members:**
**Professor Pier Champagne – pier.a.champagne@njit.edu**
**Professor Farnaz Shakib – farnaz.a.shakib@njit.edu**