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Type: **Invited talk (plenary/keynote)**

## **MODELLING ADVANCED MATERIALS WITH HIGH PERFORMANCE COMPUTING**

*Monday, 4 December 2017 11:00 (30 minutes)*

Modelling and simulation are now essential and increasingly important techniques in materials science. We aim to show the scope and challenges of the current field by reviewing recent work of the UK High End Computing Materials Chemistry Consortium. We will describe recent applications using both force-field and electronic structure techniques to key functional materials, including catalytic systems, materials for renewable energy technologies, electronic materials, ceramics and molecular materials. We will consider some of the future prospects and developments in the field.

### **HPC content**

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