



Contribution ID: 101

Type: **Invited Talk**

Molecular simulations for material optimization

Wednesday, 30 November 2022 10:15 (30 minutes)

In this talk I'll discuss how molecular dynamics and multiscale modelling can be used to accelerate material discovery and optimisation. I'll give an introduction to the techniques and HPC requirements and show two examples where molecular modelling has helped to optimize fillers composition for polymer composites and electrolytes for energy storage applications.

Primary author: Prof. CARBONE, Paola (The University of Manchester)

Presenter: Prof. CARBONE, Paola (The University of Manchester)

Session Classification: HPC Applications

Track Classification: Computational Chemistry