Contribution ID: **36** Type: **not specified**

[Remote] Machine learning and electronic structure calculation in materials and beyond

Tuesday 15 October 2024 11:20 (35 minutes)

I will briefly outline the huge importance of density functional theory (DFT) calculations to modern materials design (and to chemistry and warm dense matter, etc). I will then discuss the impact of machine learning on the field, especially the rise of machine-learned potentials. I will briefly mention my own work in using ML to improve DFT.

Focus areas

Presenter: BURKE, Kieron

Session Classification: Invited talks