Contribution ID: **370** Type: **Talk**

ChemShell: defects in energy materials by hybrid QM/MM approach

Wednesday, 3 December 2025 13:50 (20 minutes)

The presentation showcases recent developments and applications of the ChemShell software in the field of energy materials by the Materials Chemistry HPC Consortium (UK), focusing on defect properties. This work capitalizes on the software engineering and methodological advances in recent years (including the UK Excalibur PAX project highlighted in the last year CHPC conference) by the groups of Prof. Thomas W. Keal in STFC Daresbury Laboratory (UK) and Prof. C. Richard A. Catlow at UCL and Cardiff University with several collaborators. Materials of interest include wide gap semiconductors used in electronic and optoelectronic devices as well as catalysis and solid electrolytes. The method allows one to explore both defect thermodynamics and their spectroscopic properties. Further examples show how a classical rock-salt structured insulator MgO can be usefully employed as a platform in studies of exotic states of matter, which are of fundamental interest, in particular, the unconventional cuprate superconductors with high critical temperatures, and the recently discovered phenomena in isostructural nickelate systems.

Presenting Author

Alexey A. Sokol

Email

a.sokol@ucl.ac.uk

Student or Postdoc?

No. Not a student nor Postdoc.

Institute

University College London

Registered for the conference?

Yes

CHPC User

Yes

CHPC Research Programme

Workshop Duration

Primary author: Dr SOKOL, Alexey A. (University College London)

Co-authors: Prof. KEAL, Thomas (STFC); CATLOW, Richard (Department of Chemistry, University College London)

Presenter: Dr SOKOL, Alexey A. (University College London)

Session Classification: HPC Applications

Track Classification: Computational Chemistry