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Materials Modelling Workshop using Density Functional Theory (DFT)

Sunday, 30 November 2025 13:30 (1h 30m)

The Materials Modelling Workshop using Density Functional Theory (DFT) provides postgraduate students, early-career researchers, and interdisciplinary scientists with a solid foundation in computational materials science. DFT is a powerful quantum mechanical method for predicting the structural, electronic, optical, and magnetic properties of materials, enabling the rational design of novel systems for energy, catalysis, and optoelectronic applications. Through a combination of lectures and hands-on sessions, participants will gain practical experience with leading DFT software tools, learning how to perform structure optimization, electronic structure calculations, and property analysis. The workshop will highlight applications in sustainable energy materials, topological systems, and low-dimensional materials. Participants will also be introduced to emerging approaches that combine DFT with machine learning for accelerated materials discovery and inverse design. By the end of the workshop, attendees will possess both theoretical insight and computational skills to apply DFT (CASTEP in materials studio) techniques effectively in their own research and to contribute to innovation in materials design and development.

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Student or Postdoc?

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Registered for the conference?

Yes

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