

CONDENSED MATTER PHYSICS SEMINAR

Thursday 5 November at 14:30

Simpkins Lee Seminar Room, Department of Physics

(<https://maps.app.goo.gl/WjG71uLF2D48n85B6>)

From Disordered Semiconductors to AI-Driven Computational Physics

Dr. Roderick MacKenzie

University of Durham

Over the past 20 years, computational modelling of disordered semiconductors has evolved considerably, driven by advances in physical models, numerical methods and computational resources. In this talk, Roderick MacKenzie will discuss this evolution through the development of OghmaNano, a multiphysics simulation platform for semiconductor devices.

Starting with early work on molecular dynamics and quantum chemistry, the talk will move quickly to the development of drift-diffusion models incorporating trap states, enabling efficient simulation of charge transport and recombination in disordered semiconductors. The discussion will then extend to more complex device architectures, including light-emitting field-effect transistors (LEFETs), and the challenges of scaling simulations to large-area devices.

Finally, the talk will explore recent developments in AI-driven computational physics, including machine learning techniques for extracting physical parameters from experimental data and device simulations, and the use of Fourier neural networks to accelerate three-dimensional morphology simulations.

Together, these developments illustrate how computational semiconductor physics has progressed from microscopic descriptions of materials towards integrated, multiscale simulation frameworks, and how emerging AI techniques may further extend their capabilities.