

CONDENSED MATTER PHYSICS COLLOQUIUM

Thursday 21 May at 14:30

Simpkins Lee Seminar Room, Department of Physics

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Materials from first principles

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Materials underpin many of the technologies that drive our economy and sustain our societies. Providing reliable, predictive descriptions of their behaviour from first principles remains a defining challenge for condensed-matter physics and materials science — one made increasingly urgent by the convergence of high-performance computing, machine learning, and artificial intelligence, which are transforming the scale and scope of materials design and discovery.

I will discuss recent progress along three directions. First, I will address predictive accuracy, focusing on functional theories of the spectral density to address electronic excitations and correlations.

Second, I will consider realistic complexity, introducing mesoscopic transport theories that bridge microscopic equations and macroscopic diffusion. Third, I will discuss materials informatics, emphasizing automation, agency, and autonomy in campaigns of materials discovery.

These ideas will be illustrated with three case studies: the Mott–Hubbard and charge-transfer regime of transition-metal monoxides; hydrodynamic heat transport in bulk compounds and micro-devices; and in charting the electronic structure of experimentally known inorganics, searching for novel properties and improved performance.