Fall 2025 Lange Lecture
Materials Department

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University of Cambridge

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What can materials modelling do for you?

In 1929, Paul Dirac wrote that "the underlying physical laws for the mathematical theory of a large part of physics and the whole of chemistry are completely known", referring to the fact that quantum mechanics, which had just been developed, provides the framework to understand any system made of atoms. He went on to write "the difficulty is that the exact application of these laws leads to equations much too complicated to be soluble [and] it becomes desirable that approximate practical methods of applying quantum mechanics should be developed". Dirac was writing before the invention of the transistor, but now, thanks to modern computers, we can make much progress in fulfilling his vision.

Density functional theory and related methods have become extremely successful at describing simple systems at moderate computational cost. Interest in now shifting towards more challenging systems, for example materials with structural complexity and materials containing heavy ions with active d and f electrons. Together with advances in machine learning, we are reaching a point where atomistic materials modelling is becoming increasingly predictive for many systems of experimental interest.

In this lecture, I will ask the question: what can materials modelling do for you? Using examples from our recent work, I will describe how materials modelling can help rationalize increasingly complex experimental results and how materials modelling can make new predictions to guide experimental developments. Examples will span a broad range of topics, including superconductors, semiconductors, and topological materials, stressing the importance of an ongoing dialogue between experiment and computation.

Bio

Bartomeu Monserrat is Professor of Materials Physics at the Department of Materials Science and Metallurgy of the University of Cambridge. He obtained a MSci in Physics from Imperial College London in 2011 and a PhD in Physics from the University of Cambridge in 2015. He then held research positions at Rutgers University (2015-17) and Cambridge (2015-19) and joined the faculty at Cambridge in 2020.

Bartomeu leads a research group that develops and uses computational tools based on quantum mechanics to discover new materials. His work spans a wide range of materials and phenomena, including topological materials, superconductors, semiconductors for optoelectronic applications, and materials under extreme pressure conditions. His scientific contributions have been recognized with multiple awards, highlighting the international Psi-K Volker Heine Young Investigator Award, the Maxwell Medal and Prize by the UK Institute of Physics, the Young Investigator Award in Theoretical Physics by the Spanish Royal Society of Physics, and the Philip Leverhulme Prize in Physics.

Beyond research, Bartomeu is the creator and co-host of a YouTube channel teaching quantum mechanics to a global audience. The channel has over 28,000 active students and has received more than 1.8 million views.

https://www.msm.cam.ac.uk/people/monserrat

Hosted by Chris Van de Walle.