**Department of Physics**
Condensed Matter Physics
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UNIVERSITY OF OXFORD

# CONDENSED MATTER SEMINAR

Thursday 15 June at 14:30
Lindemann Lecture Theatre

## "Computational materials design with machine learning: focus on perovskites"

Prof. Dr. Silvana Botti
University of Jena

Perovskite materials have attracted increasing attention in multiple application areas thanks to their chemical diversity and extraordinary variety of electronic properties. Perovskite solar cells are the fastest advancing photovoltaic technology today. However, a large-scale application is hampered by open problems that still delay their market entry.

How can the design of functional materials - with a focus on perovskite materials - be accelerated using supercomputers? In this talk, I will discuss how first-principles calculations and machine learning can be combined to accelerate the discovery of new materials.

However, characterising the electronic properties of bulk crystalline materials may be insufficient to assess their suitability for applications, as interfaces are, after all, at the heart of electronic devices. I will conclude therefore discussing some recent progresses in the computational design of functional interfaces.

*Host: Michael Johnston*