**Department of Physics**
Condensed Matter Physics
Clarendon Laboratory, Parks Road, Oxford OX1 3PU

UNIVERSITY OF OXFORD

# CONDENSED MATTER PHYSICS SEMINAR

Thursday 26 February at 14:30
Simpkins Lee Seminar Room, Department of Physics
(https://maps.app.goo.gl/WjG71uLF2D48n85B6)

## Machine Learning-Accelerated Discovery of High-Temperature Superconductors

Professor Miguel Marques
University of Bochum

We present Alexandria, the largest academic database of calculated materials properties for inorganic solids, and demonstrate its application to the discovery of high-temperature conventional superconductors. The construction of Alexandria relies heavily on the massive acceleration provided by recent machine learning methods. This database serves as a training dataset for developing predictive models across multiple materials properties, such as universal machine-learning interatomic potentials or structure-property relationships. One such property is the transition temperature (Tc) of conventional superconductors. Using our trained models, we screened a chemical space of 160 million compounds, including both experimentally synthesized materials and theoretical structures, to identify promising candidates for high-Tc superconductivity. For the best candidates, we performed rigorous density-functional perturbation theory calculations to determine phonon spectra, electron-phonon coupling, and superconducting transition temperatures. This validation effort has yielded over 35,000 first-principles calculations, providing the most comprehensive computational survey of conventional superconductivity to date. This enables a systematic understanding of phonon-mediated superconductivity and allows us to establish definitive constraints on the maximum achievable Tc at ambient pressure. We conclude by discussing broader implications for the role of artificial intelligence in accelerating materials discovery and advancing fundamental understanding in materials science.

*Host: Professor Amalia Coldea*