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

UNIVERSITY OF OXFORD

CONDENSED MATTER PHYSICS SPECIAL SEMINAR

Monday 30 September at 14:00
Simpkins Lee seminar room

'Modern machine learning approaches for the discovery of novel high-Tc and high-Hc superconductors'

Dr. Benjamin Geisler
Department of Physics, University of Florida,
Department of Materials Science and Engineering,
University of Florida

Predicting the critical temperature Tc of a superconductor is a notoriously difficult task, even for the relatively well-understood electron-phonon-paired superconductors. The rise of machine learning introduced new computational techniques that offer a route to address this challenge.

In the first part, I will present recent advances we made in this field [1,2]. Symbolic regression employing the sure independence screening and sparsifying operator (SISSO [3]) successfully revised the functional form of the superconducting critical temperature originally proposed by McMillan, Allen, and Dynes. In conjunction with Eliashberg theory, this approach considerably enhances the accuracy of Tc prediction for conventional superconductors, which particularly also comprises the high-pressure hydrides.

Subsequently, we discuss the complementary strategy of predicting the entire electron-phonon spectral function α2F(ω) exclusively from the crystal structure, employing our recently developed Bootstrapped Ensemble of Tempered Equivariant graph neural NETworks (BETE-NET) architecture [4]. Finally, an outlook towards future research is provided, comprising our current efforts towards establishing a foundational multimodal AI for the design of high-Hc superconductors.

[1] S. R. Xie, G. R. Stewart, J. J. Hamlin, P. J. Hirschfeld, and R. G. Hennig, Phys. Rev. B 100, 174513 (2019)
[2] S. R. Xie, Y. Quan, A. C. Hire, B. Deng, J. DeStefano, I. Salinas, U. Shah, L. Fanfarillo, J. Lim, J. Kim, G. R. Stewart, J. J. Hamlin, P. J. Hirschfeld, and R. G. Hennig, npj Computational Materials 8, 14 (2022)
[3] R. Ouyang et al., Phys. Rev. Materials 2, 083802 (2018)
[4] J. B. Gibson, A. C. Hire, P. M. Dee, O. Barrera, B. Geisler, P. J. Hirschfeld, and R. G. Hennig, arXiv:2401.16611 [cond-mat.supr-con]

Host: Prof Amalia Coldea & Prof Peter Hirschfeld