

Special Condensed Matter Theory Seminar

- Subject: **Superconductivity in infinite-layer nickelates and beyond: From density functional theory to machine learning**
- Speaker: **Dr. Benjamin Geisler (University of Florida, Gainesville/USA)**
- Date & time: **Monday, 22nd of May 2023 at 3:15 p.m.**
- Venue: **Room 01.114**
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Abstract:

The recent discovery of superconductivity in NdNiO₂ films on SrTiO₃(001) has sparked significant interest in infinite-layer nickelates [1]. In the first part of my talk, I will discuss the pronounced impact of Rashba spin-orbit interactions on the surface and interface electronic structure in infinite-layer NdNiO₂/SrTiO₃(001) and NdNiO₂/KTaO₃(001) film geometries, which may result in local modifications of the pairing mechanism [2]. Subsequently, we will see how the concerted effort of experiment and theory unravels a surprising interface composition in NdNiO₂/SrTiO₃(001) that ultimately supports the notion of nickelate superconductivity as novel quantum phase, induced in film geometry by electronic reconstruction [3]. In the second part, I will present our most recent advances in predicting the superconducting critical temperature T_c , which 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 routes towards addressing this challenge, and I will discuss different approaches ranging from symbolic regression to deep learning of the Eliashberg spectral function [4,5].

[1] D. Li *et al.*, Nature **572**, 624 (2019)

[2] B. Geisler, arXiv:2303.00717 [cond-mat.supr-con] (2023)

[3] B. H. Goodge, B. Geisler, K. Lee, M. Osada, B. Y. Wang, D. Li, H. Y. Hwang, R. Pentcheva, and L. F. Kourkoutis, Nature Materials **22**, 466 (2023)

[4] S. R. Xie, G. R. Stewart, J. J. Hamlin, P. J. Hirschfeld, and R. G. Hennig, Phys. Rev. B **100**, 174513 (2019)

[5] 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 Comput. Mater. **8**, 14 (2022)

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