TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR FESTKÖRPERPHYSIK
Institute of Solid State Physics

Wiedner Hauptstr. 8-10/138, 1040 Wien
www.ifp.tuwien.ac.at

# EINLADUNG zum IFP-SEMINAR

## Core-level x-ray spectroscopy of infinite-layer nickelate: DFT+DMFT analysis

**Atsushi HARIKI**

Department of Physics and Electronics, Osaka Prefecture University,
Sakai, Osaka 599-8531, Japan

Host: Jan Kunes

Termin: Mittwoch, 30. Juni 2021, 13 Uhr CEST

Ort: via ZOOM,
https://tuwien.zoom.us/j/99253224315?pwd=b1owczZBbGtkUUhvT0tqNHJTM2Ridz09

Abstract:

Recently superconductivity was discovered in infinite-layered nickelate ($Nd_{0.8}Sr_{0.2}NiO_2$) [1]. Motivated by recent experiments for the nickelate [2,3,4], we theoretically investigate Ni 2*p* core-level x-ray photoemission spectroscopy (XPS), Ni 2*p* core-level x-ray absorption spectroscopy (XAS) and Ni 2*p*-3*d* resonant inelastic x-ray scattering (RIXS). We employ a framework based on density functional theory (DFT) and dynamical mean-field theory (DMFT) which was developed recently [5,6]. This method incorporates realistic bands (Ni 3*d*, O 2*p* and Nd 5*d* bands) with the electronic correlation and a core-valence interaction in the XPS, XAS and RIXS processes. Thus, it allows us to study spectral features beyond a conventional simple impurity-model description (e.g., cluster model or atomic model).

From the Ni 2*p* XPS analysis for $NdNiO_2$ [2], we find that Ni ion is close to the monovalent, i.e. $3d^9$ configuration in the ground state, which is reminiscent of cuprates. However, the charge-transfer energy Δ, that is the key parameter for the character of the doped hole, is larger (about 2~3 eV) than typical Δ values of cuprates. Thus, $NdNiO_2$ is somewhere between the charge-transfer and Mott-Hubbard system in the Zaanen-Sawatzky-Allen classification. Besides only the Ni $x^2$-$y^2$ orbitals are partially filled and multiorbital physics does not play an important role for the stoichiometric as well as slightly hole-doped compound. The Ni 2*p* XAS and RIXS analysis [3,4] supports this conclusion. We find that self-doping from the Nd 5*d* states in the vicinity of the Fermi energy prohibits opening of Mott-Hubbard gap in $NdNiO_2$.

[1] D. Li et al., Nature **572** 624 (2019)
[2] Y. Fu et al., arXiv:1911. 03177 (2019)
[3] M. Hepting et al., Nat. Mat. **19**, 381 (2019)
[4] M. Rossi et al., arXiv:2011: 00595 (2020)
[5] A. Hariki et al., Phys. Rev. B **101**, 115130 (2020)
[6] A. Hariki et al., Phys. Rev. Lett. **121**, 126403 (2018)