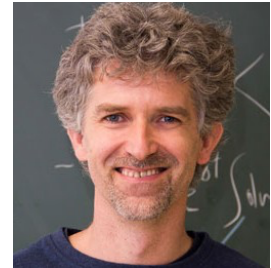


# Jan Kunes

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**Tuesday, 23<sup>th</sup> March 2021, 16:00 s.t.**

The seminar will be held as a Zoom Meeting

<https://tuwien.zoom.us/j/96062751637?pwd=ZkRUWnlkUFFZb2pEdm5ZzFteTBNdz09>

Meeting ID: 960 6275 1637 Passcode: 9ANd8XWj



## Core-level spectroscopy of transition metal oxides

Improving energy resolution of core-level photoemission (XPS) experiments in the past ten years has led to the realization that valuable information about the valence electronic structure can be obtained by this seemingly atomic probe. Similar improvements in resonant inelastic x-ray scattering (RIXS) made this originally chemists' tool (eV scale) a precious part of physicists' toolkit (10 meV scale). I will present a computational approach for simulation of core-level spectra based on combination of dynamical mean-field theory with a postprocessing using a specially tailored exact diagonalization method. I will discuss applications of this approach to the calculation of XPS, RIXS and x-ray absorption spectra of selected transition metal oxides such as  $\text{LaCoO}_3$ ,  $\text{V}_2\text{O}_3$  or monoxides  $\text{NiO}$  and  $\text{MnO}$ .

All interested colleagues are welcome to this seminar lecture  
(30 min. presentation followed by discussion).

Friedrich Aumayr  
(LVA-Leiter)

Ulrike Diebold  
(Seminar Chair)

A Joint Seminar with SFB F81 TACO