LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN | ARNOLD SOMMERFELD CENTER FOR THEORETICAL PHYSICS

Sommerfeld Theory Colloquium

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Effects of electronic correlations in BaOsO3 and tetragonal CuO

Strongly correlated electron systems, i.e. systems where the interaction between electrons cannot be treated as an effective potential, are an extremely fascinating, but also very challenging topic in modern solid state physics. The challenge arises in parts due to the simultaneous importance of non-local kinetic and local correlation effects, which make it important to treat both at equal footing. For this reason Dynamical Mean Field Theory (DMFT) has in the last decades become the state of the art method for electronic structure caluclations of strongly correlated electrons as it includes local correlation effects exactly, but also respects kinetic effects in terms of an embedding approach. In this talk, we will first motivate our interest in strongly correlated materials by giving an example regarding the fascinating properties that these materials can exhibit. This will be followed by an intuitive introduction to DMFT. Finally we present results from our DMFT studies of two strongly correlated systems: BaOsO3 [1] and tetragonal CuO (t-CuO) [2].

[1] MB, Jernej Mravlje, Martin Grundner, Ulrich Schollwöck, and Manuel Zingl, Phys. Rev. B. 103, 165133 (2021)

[2] MB, B. Bacq-Labreuil, M. Grundner, S. Biermann, U. Schollwöck, S. Paeckel, and B. Lenz, SciPost Phys., 14, 010 (2023)

Wednesday, 20 December 2023, 16:15h, Room A348, Theresienstr. 37/III

Prof. Uli Schollwöck