Minicolloque n°21 Oral

BaOsO₃: A Hund's metal in the presence of strong spin-orbit coupling

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(Dated: May 10, 2021)

Hund's metals are a class of material which have recently drawn a lot of attention. The interorbital Hund's coupling J_H in these materials leads to important electronic correlation effects despite the fact, that J_H is usually only 10-20% of the intra-orbital Hubbard repulsion U. So far the effects of spin-orbit coupling (SOC) in Hund's metals have for example been studied in the context of Sr_2RuO_4 and Sr_2MoO_4 , however while the interplay with electronic correlations gave rise to a static effective enhancement of SOC, one did not observe any influence on dynamical quantities. In order to learn more about the interplay between SOC and Hund's metal physics we therefore study $BaOsO_3$ a 5d transition metal oxide with 4 electrons in the t_{2g} shell similar to ruthenates but with stronger SOC ($\lambda = 0.3 \, \text{eV}$) using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We find that $BaOsO_3$ can be best pictured as a moderatley correlated Hund's metal in which the physics is governed by an intriguing interplay of SOC, Hund's coupling J_H and a van-Hove singularity (vHs) close to the Fermi level.

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