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

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Hund’s metals are a class of material which have recently drawn a lot of attention. The inter-orbital 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 Sr₂RuO₄ and Sr₂MoO₄, 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 BaOsO₃ a 5d transition metal oxide with 4 electrons in the $t_{2g}$ shell similar to ruthenates but with stronger SOC ($\lambda = 0.3$ eV) using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). We find that BaOsO₃ can be best pictured as a moderately 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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