European XFEL Theory Seminar

Wednesday 10th of July 2019, 16:00
Campus Schenefeld, main building (XHQ) room E1.172

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Osmates on the verge of a Hund's-Mott metal-insulator transition: The different fates of $NaOsO_3$ and $LiOsO_3$

In this talk, I will discuss how a delicate interplay of correlation effects can explain the strikingly different spectroscopic properties of the chemically similar compounds $NaOsO_3$ and $LiOsO_3$. In particular, our first-principle many-body analysis (based on DFT+ DMFT) demonstrates that the physics of the high-temperature paramagnetic phases of these two 5d transition metal oxides is controlled by the presence of an adjacent Hund's-Mott insulating phase. Minor differences between the materials result in a tremendously sharp change of the electronic mobility, hence explaining the untypically different high-temperature properties.

At the same time, while the (sizable) spin-orbit coupling (SOC) does not affect significantly the paramagnetic properties, our preliminary many-body calculations including SOC show that its role could be indeed crucial, in the low-temperature regimes, to explain the qualitatively different magnetic behavior of the two materials.

Host: Evgeny Gorelov