Electronic correlations in $V_2(Te,Se)_2O$: A DFT+DMFT study

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Electron-electron interactions are widely accepted the underlying physical mechanism explaining the diversity of unusual fermionic states in quasi-two-dimensional materials. Recently, a new class of correlated van der Waals oxychalcogenides, including V_2Te_2O [1] and V_2Se_2O [2], has been synthesized. These materials exhibit unusual properties including anomalous log(1/T) temperature dependence of resistivity, correlation-induced localization effects and significant electron-mass renormalization, that cannot be explained within the picture of weakly interacting electrons implying a significant role of Coulomb correlation effects.

In this work, we explore the effect of Coulomb correlations on the electronic structure of V_2Te_2O and V_2Se_2O using a computational framework combining density functional theory (DFT) and dynamical mean-field theory (DMFT). In V_2Te_2O, Coulomb correlations induce significant quasiparticle mass renormalization for the vanadium $3d$ states, offering an improved description of the Sommerfeld coefficient [3]. For V_2Se_2O, it drives a critical redistribution of spectral weight at the Fermi level, leading to a gap opening in the electronic spectrum, consistent with experiments. These findings suggest V_2Se_2O behaves as a correlation-assisted Slater insulator and highlight the pivotal role of Coulomb correlations in shaping the electronic properties of both materials. This work was supported by the Russian Science Foundation (project no. 24-12-00024).

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