

Thermopower in strongly correlated Sr_2RuO_4 from first principles

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Sr_2RuO_4 is a correlated metal with the specific heat enhancement about 4 times over the LDA value. NMR and ARPES measurements reveal the crossover to incoherent regime at about 100K. Remarkably, quantum oscillations reveal larger mass enhancement of the carriers in the widest band. We analyze Sr_2RuO_4 within LDA+DMFT, which reproduces and explains these experimental observations. The low coherence scale and the anomalous mass renormalizations are related to the Hund's rule coupling and to the proximity to the van Hove singularity [1]. Encouraged by good agreement with experiment, we calculated also the transport quantities. The dependence of Seebeck coefficient on temperature is reproduced well. The semi-saturation which occurs above 150K is related to the crossover to the incoherent regime. Our results demonstrate LDA+DMFT method is promising for investigation of thermopower in correlated electron systems.

[1] Jernej Mravlje, Markus Aichhorn, Takashi Miyake, Kristjan Haule, Gabriel Kotliar, and Antoine Georges, *Phys. Rev. Let.* **106**, 096401 (2011).