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Transport properties of correlated metals: A dynamical mean field theory perspective[1]

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Strongly correlated metals, including many transition metal oxides, are characterized by unconventional transport properties with anomalous temperature dependence. For example, in many systems Fermi liquid behavior holds only below an extremely low temperature while at high temperature these bad metals have large resistivity which exceeds the Mott-Ioffe-Regel (MIR) limit. Material specific calculation of these anomalous transport properties is an outstanding challenge. Recent advances enabled us to study the transport and optical properties of two archetypal correlated oxides, vanadium oxides and ruthenates, using the LDA+DMFT method. In V2O3, the prototypical Mott system, our computed resistivity and optical conductivity are in very good agreement with experimental measurements, which clearly demonstrates that the strong correlation dominates the transport of this material [4]. Furthermore by expressing the resistivity in terms of an effective plasma frequency and an effective scattering rate, we uncover the so-called "hidden Fermi liquid" [1, 2, 3] behavior, in both the computed and measured optical response of V2O3. This paradigm explains the optics and transport in other materials such as NdNiO3 film and CaRuO3. In the ruthenates family, we carried out a systematical theoretical study on the transport properties of four metallic members, Sr2RuO4, Sr3Ru2O7, SrRuO3 and CaRuO3, which generally encapsulates the gradually structure evolution from two-dimension to three dimension. With a unified computational scheme, we are able to obtain the electronic structure and transport properties of all these materials [5]. The computed effective mass enhancement, resistivity and optical conductivity are good agreement with experimental measurements, which indicates that electron-electron scattering dominates the transport of ruthenates. We explain why the single layered compound Sr2RuO4 has a relative weak correlation with respect to its siblings, which corroborates its good metallicity. Comparing our results with experimental data, benchmarks the capability as well as the limitations of existing methodologies for describing transport properties of realistic correlated materials. [1] Xiaoyu Deng, Jernej Mravlje, Rok Zitko, Michel Ferrero, Gabi Kotliar, Antoine Georges, Physical Review Letters, 110, 086401 (2013). [2] Christophe Berthod, Jernej Mravlje, Xiaoyu Deng, Rok Zitko, Dirk van der Marel, and Antoine Georges, [3] Phys. Rev. B, 87, 115109 (2013) Wenhu Xu, Kristjan Haule, and Gabriel Kotliar, Physical Review Letters, 111, 036401(2013) [4] Xiaoyu Deng, Aaron Sternbach, Kristjan Haule, D. N. Basov, Gabriel Kotliar, Physical Review Letters, 113, 246404 (2014) [5] Xiaoyu Deng, Kristjan Haule, Gabriel Kotliar, Physical Review Letters, 116, 256401 (2016).

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