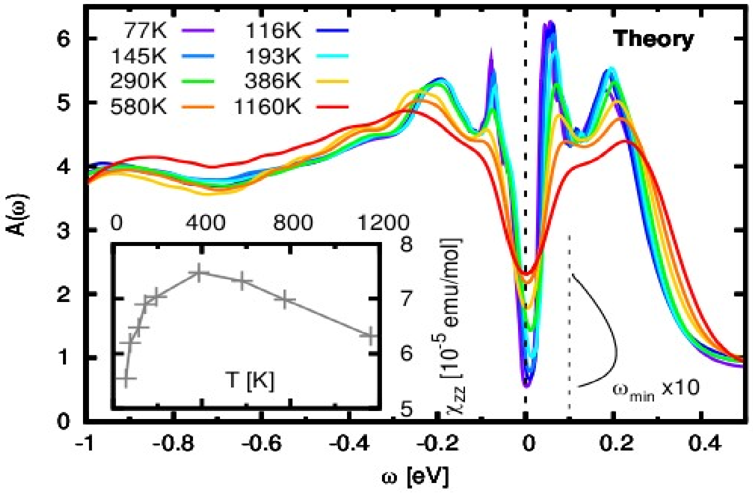
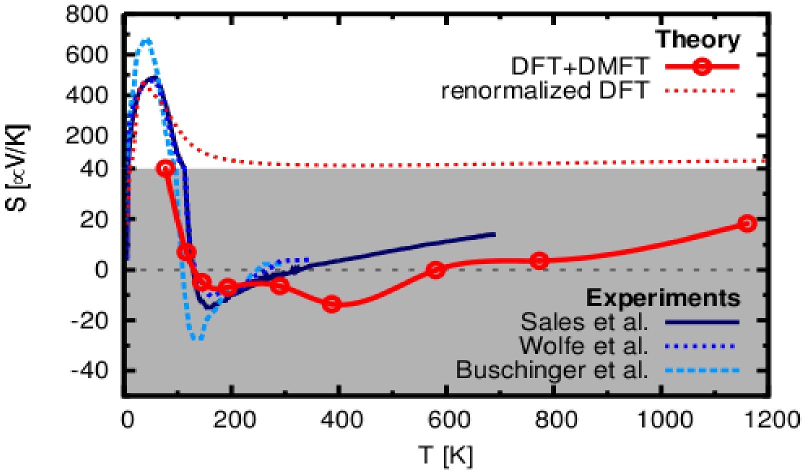
Large thermoelectric power in FeSi, a strongly correlated semiconductor

Kristjan Haule, Jan Tomczak & Gabriel Kotliar,
Rutgers The State University of New Jersey

The intermetallic FeSi exhibits an unusual temperature dependence in its electronic and magnetic degrees of freedom, epitomized by the enormous thermoelectric power, and a crossover from a low temperature non-magnetic semiconductor to a high temperature paramagnetic metal with a Curie-Weiss susceptibility. Using the realistic many-body calculations, we reproduce the signatures of the metal insulator transition in various observables: the spectral function, the optical conductivity, the spin susceptibility, and the Seebeck coefficient. Drawing from the microscopic insights of our approach, we show how the spin spin excitations at finite temperature can destroy the semiconducting gap in a narrow gap semiconductor, and how the resulting metallic state achieves a very large thermoelectric power through the correlation induced incoherence.





Left: Theoretical one particle density of states of FeSi for various temperatures shows how magnetic excitations cause a collapse of the semiconducting gap.

Right: Theoretical optical conductivity for FeSi and comparison with experiment.

Right: The change in the effective number of carriers with temperature from theory and experiment. The effective number of carriers is proportional to the integral of the optical conductivity. It is a measure of the energy redistribution of spectral weight.
Left:
Temperature dependence of the thermoelectric power explained by theoretical method, both the low temperature and the intermediate temperature range, including the double sign change with increasing temperature.