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Enhancement of the $Na_{0.7}CoO_2$ thermopower due to electronic correlations

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The merger of the local density approximation (LDA) and dynamical mean field theory (DMFT) has been a breakthrough for the calculation of materials with strong electronic correlations such as transition metal oxides and heavy fermion systems [1]. The reason for this success is that local correlations are the major ones, at least for these kinds of strongly correlated materials.

After a brief introduction to the method, I will show how electronic correlations increase the thermopower of $Na_{0.7}CoO_2$ by 200%. The newly revealed mechanism [2] is an asymmetric shift of (quasi) electrons and holes away from the Fermi level, concurrent with an asymmetry of the respective (group) velocities. Exploiting this effect in bandstructure and correlation engineering may lead to a substantial increase of the thermoelectric figure of merit.

Besides, I would like to briefly discuss the dichotomy between large theoretical and small experimental moments in iron pnictides [3] and, as an outlook into the future development, discuss a route to include non-local correlations beyond DMFT. This allows us,. e.g., to calculate the critical exponents of the Hubbard model in two and three dimensions [4].

[1] For a recent review see K. Held Adv. Phys. **56**, 829 (2007).
[2] P. Wissgott et al. Phys. Rev. B **82**, 201106 (2010);
arXiv:1105.3841 <http://arxiv.org/abs/1105.3841>.
[3] P. Hansmann et al. Phys. Rev. Lett. **104**, 197002 (2010).
[4] G. Rohringer et al., arxiv.org/abs/1104.1919.