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Oxide heterostructures: from efficient solar cells to quantum anomalous Hall states

Heterostructures made of transition metal oxides are an emerging class of materials which may replace at some point conventional semiconductors for specific applications. We have developed a density functional theory plus dynamical mean field theory (DFT+DMFT) approach for such heterostructures. This allows for treating strong electronic correlations which are of fundamental importance for many transition metal oxides.

First, I will show how to exploit the unique properties of oxide heterostructures for high-efficiency solar cells [1]: The intrinsic electric field of polar heterostructures allows for efficiently separating the created electrons and holes. Our proposed solar cell has been realized experimentally [2] which also proves the existence of a polar field. Here, electronic correlations can be useful: impact ionization [3,4] can increase the efficiency of the solar cell which may help to overcome the Shockley-Queisser limit of 38% efficiency.

Besides, I will discuss the difficulties in making ultrathin ferromagnetic films and how to overcome it through SrRuO₃ heterostructures grown in the (111) direction. For a bilayer, these heterostructures even host Haldane's quantum anomalous Hall state [5].

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[3] P. Werner, K. Held, and M. Eckstein, Phys. Rev. B 90, 235102 (2014).

[4] M. E. Sorantin et al., arXiv:1708.05011.

[5] L. Si et al., Phys. Rev. Lett. 119, 026402 (2017)