Prof. Dr. Karsten Held

TU Wien

Oxide heterostructures: from efficient solar cells to spin-orbit coupling

Heterostructures made of transition metal oxides are 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.
In the first part, I will show how to exploit the unique properties of these heterostructures for high-efficiency solar cells [1]: The intrinsic electric field of polar heterostructures allows forefficiently separating the created electrons and holes. Furthermore, the heterostructure naturally provides electrical contacts through ultra-thin conducting interface layers. The bandgap in some heterostructures is optimal for the solar spectrum and can be tuned by using different chemical elements layer-by-layer. Last but not least electronic correlations can give rise to impact ionization [2] and may hence help to overcome the Shockley-Queisser limit of 39% efficiency.
In the second part, I will present the theory of spin-orbit coupling in oxide heterostructures [3] which, due to multi-orbital effects, is strikingly different from the standard Rashba theory of semiconductor heterostructures: By far the biggest effect is at the crossing point of the xy and yz orbitals. The coupling to a ferroelectric material may boost the Rashba spin splitting to room temperature energy scales [4].

[1] E. Assmann et al., Phys. Rev. Lett. 110, 078701 (2013).
[2] P. Werner, K. Held, and M. Eckstein, Phys. Rev. B 90, 235102 (2014).
[3] Z. Zhong, A. Toth, and K. Held, Phys. Rev. B 87, 161102(R) (2013).
[4] Z. Zhong, L. Si, Q. Zhang, W.-G. Yin, S. Yunoki, and K. Held, Adv. Mater. Interfaces, 1400445 (2015).