Oxide heterostructures: from superconductivity to solar cells

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Heterostructures made of transition metal oxides are an upcoming class of materials which may replace at some point conventional semiconductors for specific applications. We show how to possibly exploit the unique properties of oxide heterostructures for tailoring a Fermi surface as for high-T_C cuprates in nickelates [1] and how to engineer high-efficiency solar cells [2].

For the nickelates [1], an orbital engineering by means of heterostructuring is possible. That is, in a 1/1 LaNiO3/LaAlO3 heterostructure a single predominantly Fermi surface sheet of predominantly $x^2 - y^2$ character remains, while the Ni $3z^2 - 1$ orbital plays the role of the axial Cu 4s-like orbital in the cuprates. We put the difference between dp- [3] and d-only calculations into perspective [4].

As for the solar cells [2], the intrinsic electric field of polar heterostructures allows for efficiently separating the created electrons and holes. Furthermore, the heterostructure naturally provides electrical contacts through ultra-thin conducting interface layers. Last but not least, the bandgap in some heterostructures is optimal for the solar spectrum and can be tuned by using different chemical elements layer-by-layer.

Briefly, the theory of spin-orbit coupling in oxide heterostructures is presented [2]. Due to multi-orbital effects it 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 in case of $LaAlO_3/SrTiO_3$; and around the Γ point a spin splitting with a linear *and* cubic dependence on the wave vector $\vec{k}$ is possible.

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