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Electric field effects in transition metal oxides, their surfaces and heterostructures[1]

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Modern computational tools such as density functional theory and its merger with dynamical mean field theory are nowadays inevitable for the modeling and understanding of oxides, their heterostructures and surfaces. In this talk, I will concentrate on the impact of electric fields, how they affect the physical properties and how to make use of them. Substantial internal electric fields are created at polar surfaces, and even for an isopolar-interface the electronic reconstruction can lead to a charge transfer and hence a dipole field [1]. Such internal fields can be employed to efficiently separate electrons and holes in a oxide solar cell [2]. Even if the polar dipole field is compensated by a surface reconstruction, a local surface potential remains, and makes $SrTiO_3$ (110) the arguably simplest 2 dimensional electron gas (2DEG) [3]. External electric fields, on the other hand, can trigger "gigantic" responses, since correlated oxides are prone to small perturbations. For example, a field effect Mott transistor can be realized in a few layers of $SrVO_3$ with ideal on-off (metal-insulator) switching properties [4]; and interfacing a ferroelectric, $BaTiO_3$, plus a 2DEG with large spin-orbit coupling, $BaOsO_3$, allows for a giant switchable Rashba effect.

[1] J. E. Kleibeuker et al. Phys. Rev. Lett. (2014).
[2] E. Assmann et al., Phys. Rev. Lett. 110, 078701 (2013).
[3] Z. Wang et al, Proc. Natl. Acad. Sci. 111, 3933 (2014).
[4] Z. Zhong et al., arXiv:1312.5989.

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