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Correlated Heterostructures for Efficient Solar Cells ELIAS ASS-MANN, MARKUS AICHHORN, TU Graz, Austria, GIORGIO SANGIOVANNI, University of Würzburg, Germany, SATOSHI OKAMOTO, Oak Ridge National Laboratory, PETER BLAHA, SUMANTA BHANDARY, KARSTEN HELD, TU Vienna, Austria — Polar|non-polar oxide heterostructures such as LaAlO₃|SrTiO₃ have become well-known for the many intriguing phenomena occurring at the interface, especially the internal potential gradient and the resulting 2d electron gas. We propose to make use of these unique systems as absorbing materials for highefficiency solar cells [1]. In particular, LaVO₃|SrTiO₃ (i) has a direct band gap ~ 1.1 eV, nearly optimal for a solar cell; (*ii*) the internal potential gradient serves to efficiently separate the photo-generated electron-hole pairs and reduce recombination losses; (*iii*) the conducting interface offers a natural contact for charge-carrier extraction. Furthermore, (iv) oxide heterostructures afford the flexibility to combine layers with different gaps, e.g. LaVO₃ with LaFeO₃, in order to achieve even higher efficiencies with band-gap graded solar cells. We use density-functional theory and dynamical mean-field theory to study this strongly correlated heterostructure.

[1] Assmann et al., PRL 110, 078701 (2013)
Experimental corroboration: Liang et al., Sci. Rep. 3, 1975 (2013); Wang et al., PR Applied 3, 064015 (2015)

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