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Self-doping and emergent conductance at Mott interfaces via internal charge transfer[1] HANGHUI CHEN, ANDREW MILLIS, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Math, Columbia University — We use *ab initio* calculations to show that internal charge transfer can induce spatially separated electron-hole pairs at interfaces between two Mott insulators. DFT+ U studies of multilayer systems consisting of Sr_2VO_4 and Sr_2MnO_4 (both Mott insulators) reveal that conductance emerges at their interface with electrons residing dominantly on the Mn $d_{x^2-y^2}$ orbital and holes on the V d_{xy} orbital. With the transferred electron coupled to the core spin on Mn sites, ferromagnetism is significantly favored in the Sr_2MnO_4 layer, although this material is antiferromagnetic in bulk. Our work establishes internal charge transfer as a powerful method of tailoring correlation effects and that superlattices composed of Ruddlesden-Popper type oxides provide new possibilities for materials design, complementary to perovskite oxide heterostructures.

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