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Extreme doping in complex oxides

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Complex oxides host a wide variety of interesting physical properties, including charge localization in the form of small polarons, magnetism,ferroelectricity, giant magnetoresistance, and high-Tc superconductivity. In this presentation we discuss how doping can modify the properties of complex oxides, for instance by transforming a band insulator into a Mott insulator. We discuss results of first-principles calculations for the evolution of the electronic structure of complex-oxide heterostructures as a function of the thickness in quantum-well heterostructures. More specifically, we show how a two-dimensional electron gas becomes a Mott-insulator as the thickness of the quantum well is decreased. The onset of charge localization is analyzed in terms of electron density in octahedral distortions at the interface. We compare our results to available experimental results.

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