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Electron-electron interactions and lattice distortions in the perovskite titanates

LARS BJAALIE, University of California, Santa Barbara

A two-dimensional electron gas (2DEG) with the unprecedented high density of $3x10^{14}$ (corresponding to 1/2 electron per interface unit cell area) can be formed at the interface between $SrTiO_3$ and a rare-earth titanate ($RTiO_3$). The 2DEG resides in the $SrTiO_3$, and arises from a polar discontinuity at the interface. The formation of this 2DEG has led us to study these perovskite titanates in detail. Some of these compounds are Mott insulators, where a Mott-Hubbard gap opens up between partially filled Ti 3*d* bands. This talk focuses on the importance of the interplay between electron-electron interactions and lattice distortions in these complex oxides, which we study with density functional theory using a hybrid functional, capable of correctly describing electron localization and Mott-insulating behavior. These effects are crucial to understanding the metal-to-insulator transition as a function of electron density. Indeed, very thin $SrTiO_3$ layers inserted in $GdTiO_3$ show insulating behavior, in contrast to the metallic character of thicker layers in which the electrons form a 2DEG. The same physics is observed in bulk $SrTiO_3$ when doped with 1/2 electron per Ti atom [1]. Charge localization and lattice distortions also govern the formation of small hole polarons in the rare-earth titanates. We demonstrate that these polarons impact the optical absorption measurements commonly used to determine the value of the Mott-Hubbard gap [2].

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