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Structural and electronic defects in $SrTiO_3$ and TiO_2[1]

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Control of defects and charge carriers is key to the development of metal oxide semiconductors as electronic materials. As in any semiconductor, one of the main challenges is to control the conductivity by doping as well as to reduce the concentration of native defects and unintentional impurities that act as compensation centers or sources of deep level luminescence, thus minimizing their deleterious effects. Experiments indicate that defects such as oxygen vacancies easily form and strongly affect the electronic properties of many oxide semiconductors. In $SrTiO_3$, it has been proposed that oxygen vacancies simultaneously act as a shallow donor that contribute to n-type conductivity, and as a deep center that causes luminescence well below the band-gap energy. This seemingly paradoxical behavior has remained unresolved. In rutile TiO_2, it has been proposed that excess electrons, either from oxygen vacancies or donor impurities, form small polarons. Although the formation of small polarons explains prominent features observed in the optical absorption spectra, charge localization seem incompatible with the high electron mobilities determined in Hall measurements of single crystals. In this talk we will discuss results of first-principles calculations for native point defects and impurities in $SrTiO_3$ and TiO_2, as they are prototypes of a large class of transition-metal oxide semiconductors. We will address the impact of defects and small-polaron formation on the electrical and optical properties in each material, providing a framework for interpreting similar phenomena in other complex oxides.

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