Two-dimensional charge trapping in metal-oxide materials

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The trapping of electrons and holes in oxides is a fundamental effect critical to the performance of materials in microelectronics, energy generation, and photocatalysis. In highly polarisable oxides, electrons and holes can self-trap in the perfect lattice (i.e. polaron formation), but can also be trapped by pre-existing defects, such as impurities, surfaces and interfaces [1]. Since separating these effects in order to characterise charge trapping in real materials experimentally remains extremely challenging, theoretical models can be invaluable.

In this talk, I will give an overview of the main theoretical challenges to accurate prediction of charge trapping in oxides before presenting several examples of systems where the nature of electron and hole trapping is predicted to be two-dimensional. These will include the polaronic trapping of holes in bulk HfO_2 [2], hole trapping at the surface of ZrO_2 nanocrystals [3], and electron and hole trapping by grain boundaries in MgO and HfO_2 [4-6]. In many ways the two-dimensional properties of these systems are similar to those pronounced in numerous layered oxides as well as in 2D electron gases that can be formed at oxide heterointerfaces and in the high-Tc superconducting cuprates.

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