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Metal-induced gap states in ferroelectric capacitors and its relationship with complex band structures[1] JAVIER JUNQUERA, PABLO AGUADO-PUENTE, Universidad de Cantabria — At metal-isulator interfaces, the metallic wave functions with an energy eigenvalue within the band gap decay exponentially inside the dielectric (metal-induced gap states, MIGS). These MIGS can be actually regarded as Bloch functions with an associated complex wave vector. Usually only real values of the wave vectors are discussed in text books, since infinite periodicity is assumed and, in that situation, wave functions growing exponentially in any direction would not be physically valid. However, localized wave functions with an exponential decay are indeed perfectly valid solution of the Schrodinger equation in the presence of defects, surfaces or interfaces. For this reason, properties of MIGS have been typically discussed in terms of the complex band structure of bulk materials. The probable dependence on the interface particulars has been rarely taken into account explicitly due to the difficulties to include them into the model or simulations. We aim to characterize from first-principles simulations the MIGS in realistic ferroelectric capacitors and their connection with the complex band structure of the ferroelectric material. We emphasize the influence of the real interface beyond the complex band structure of bulk materials.

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