On the origin and switching of a two-dimensional electron gas under a thin perovskite film

N. Bristowe[1], P. Aguado-Puente[2], R. Shirasawa[3*], B. Yin[2,4], P. Littlewood[5,6], Ph. Ghosez[7] and E. Artacho [2,8,9]
1- Department of Materials, Imperial College London, London SW7 2AZ, UK
2- CIC NanoGUNE and DIPC, Tolosa Hiribidea 76, 20018 San Sebastián, Spain
3- Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, UK
4- Department of Engineering Mechanics, Zhejiang University, Hangzhou 310027, China
5- Physical Sciences and Engineering, Argonne National Laboratory, Argonne, Illinois 60439, USA
6- Department of Physics, University of Chicago, 5720 S. Ellis Ave, Chicago, IL 60637, USA
7- Département de Physique, Université de Liège, B-4000 Sart-Tilman, Belgium
8- Theory of Condensed Matter, Cavendish Laboratory, University of Cambride, J. J. Thomson Av. Cambridge CB3 0HE, UK
9- Basque Foundation for Science Ikerbasque, 48011 Bilbao, Spain

Since the discovery of the two-dimensional electron gas (2DEG) that forms at the interface between a nanoscale thin film of LaAlO3 and a SrTiO3 substrate [1], the research on this and similar systems has been very active, leading to the discovery of a vast amount of different properties with potential practical applications [2]. The origin of such a 2DEG between two band insulators has remained controversial for some time. Our present understanding, in terms of a polarization discontinuity at the interface will be briefly reviewed, connecting with concepts that are now more topically associated to topological insulators [3].

Although the formation of a 2DEG has been observed in other oxide heterostructures, the prototypical system for these studies is still the original $LaAlO_3/SrTiO_3$ interface. Very early after the discovery of this system, the use of a ferroelectric substrate was proposed as a way to tune the population of the 2DEG. Since the ferroelectric material possess a non-volatile polarization, its switching with the application of an external electric field could be used to increase or decrease the polar discontinuity with the polar $LaAlO_3$ and consequently turn on and off the 2DEG. First-principles simulations showed that this was physically feasible [4] but the experimental realization has not been achieved yet. A more radical approach to this problem considers the spontaneous polarization of a ferroelectric material instead of the formal polarization of the centrosymmetric $LaAlO_3$, suggesting that a 2DEG should also form under ferroelectric thin films due to a polarization discontinuity with a dielectric substrate or vacuum. If this were achieved a number of possible applications can be envisaged, such as non-volatile manipulation of the metallic interface. Here we present a combination of macroscopic models and first principles simulations aimed at explaining the precise conditions under which the formation of a 2DEG under a ferroelectric thin films might be viable and what the properties of the system would be. We study the competition between the electronic reconstruction and typical alternative screening mechanisms, paying special attention to the formation of polydomain structures. These results are used to propose routes to favor the formation of the 2DEG. The properties of the 2DEG formed at realistic ferroelectric surfaces or interfaces are analyzed using first principles simulations, taking explicitly into account the interaction with the substrate, the external fields, strain, and other instabilities present in the materials. The switching on and off of the 2DEG is obtained in the modeling and the calculations, displaying a discontinuity in the polarization and in the corresponding screening mechanism (the free carriers of the 2DEG) equal to $P_s / \sqrt{3}$, P_s being the equilibrium bulk polarization of the material.

* Present address: Sony Corporation, Atsugi-shi, Kanagawa 243-0021,Japan

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