

Abstract Submitted  
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**Nanoscale smoothing and the analysis of interfacial charge and dipolar densities** JAVIER JUNQUERA, MORREL H. COHEN, KARIN M. RABE, Dep. of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, PHILIPPE GHOSEZ, Dép. de Physique, Université de Liège, B-4000 Sart-Tilman, Belgium — The transfer of charge that occurs in a metal-dielectric interface is a difficult issue, whose deep understanding requires first-principles calculations. The problem then arises about how to extract from the immense detail provided by the first-principles results the physical quantities of interest. The difficulty comes from the fact that the interface-related dipole densities are overwhelmed by the much larger variations of the total microscopic charge density. Accordingly, nano-smoothing procedures have been developed <sup>1</sup> in order to localize the physically relevant charge densities to the interface. Here we discuss the criteria for validity that the smoothing procedure should meet to leave the physical quantities unaffected. We have applied the model to compute directly the polarization charge density of a realistic ferroelectric capacitor <sup>2</sup> and find it to be much smaller than the bulk ferroelectric polarization. We attribute this reduction to the penetration of the metallic wave functions into the ferroelectric, which leads to screening of the polarization charge within the ferroelectric itself. Work supported by DOE Grant DE-FG02-01ER45937

<sup>1</sup>L. Colombo *et al.*, Phys. Rev. B **44**, 5572 (1991)

<sup>2</sup>J. Junquera and Ph. Ghosez, Nature **422**, 506 (2003)

Morrel H. Cohen  
Dep. of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019

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