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Interplay between structure and electronic properties in metal-oxide interfaces MATIAS NUNEZ, MARCO BUONGIORNO NARDELLI[1], Department of Physics, North Carolina State University, Raleigh, NC 27695, USA — Using first principles calculations we have investigated a broad spectrum of metal-insulator interfaces, including crystalline oxides and ferroelectrics. In our study we have focussed on the role of the interface phase in determining the properties of the composite system and, in particular, the relation between interface structure, charge transfer at the interface, and the associated interface dipole. For crystalline oxides such as BaO or SrO, our results demonstrate the possibility of tuning the Schottky barrier height by manipulating the interface phase [1]. For ferroelectric materials, such as BaTiO3, we have analyzed the interplay between the interface phase, the thickness of the ferroelectric layer and the residual polarization of the thin film. The polarization of the ferroelectric has been computed using modern theory of polarization via the displacements of the centers of the Wannier functions associated with the system. [1] M. Nunez and M. Buongiorno Nardelli, Phys. Rev. B, 73, 235422 (2006).

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