

Abstract Submitted  
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**First principles theory of metal-oxide interfaces: the Schottky-Mott theory revisited** MATIAS NUNEZ, MARCO BUONGIORNO NARDELLI, North Carolina State University — Using calculations from first principles, we discuss the interplay between structure and functionality at metal-insulator interfaces using the paradigmatic example of the junctions between various metals (Ag, Pd,Pt,Ni,Cu,Al) and binary crystalline oxides (BaO,CaO and SrO). Our results demonstrate that it is possible to tune the Schottky barrier height in a very broad range of values just manipulating the metal at the interface and elucidate the role of the relative overlap in the density of states of the different components in determining the band alignment. We will also show how we can apply this concepts to interfaces between metals and ferroelectric oxides where the interface structure and charge transfer affect the spontaneous polarization of the ferroelectric.

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