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Unusual electronic states in TiO_2/VO_2 (001) multilayers. VICTOR PARDO, WARREN PICKETT, University of California Davis, PARDO-PICKETT COLLABORATION — Abrupt interfaces between oxides display a wealth of unexpected behavior, and the interface between a band insulator and a Mott insulator is expected to display extra richness. Several multilayered TiO_2/VO_2 structures have been studied by ab initio density functional theory techniques, including the thin VO_2 regime corresponding to the quantum confined Mott insulator. VO_2 undergoes a metal-insulator transition near room temperature, but when deposited in thin films of thickness smaller than 5 nm, the metal-insulator transition disappears. Our calculations (using the correlated LDA+U method with modest values of U and J) show that the electronic character (metallic versus insulating) changes with the number of VO_2 layers embedded within insulating TiO_2 layers: metallic for five VO_2 layers, semimetallic and half-metallic for three layers, and insulating for a single VO_2 layer. These trends, and the peculiar nature of the three VO_2 layer case, will be discussed in some detail.

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