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Unusual electronic states in TiO₂/VO₂ (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 TiO₂/VO₂ structures have been studied by ab initio density functional theory techniques, including the thin VO₂ regime corresponding to the quantum confined Mott insulator. VO₂ 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 VO₂ layers embedded within insulating TiO₂ layers: metallic for five VO₂ layers, semimetallic and half-metallic for three layers, and insulating for a single VO₂ layer. These trends, and the peculiar nature of the three VO₂ layer case, will be discussed in some detail.

Prefer Oral Session
 Prefer Poster Session

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