VO_2 and Friends: A Novel View from Band Theory

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Recent calculations for vanadium dioxide, one of the most controversely discussed materials for decades, reveal that, contrary to previous assertions, band theory as based on density functional theory is well capable of correctly describing the electronic and magnetic properties of the metallic as well as both the insulating M_1 and M_2 phases. Considerable progress in the understanding of the physics of VO_2 is achieved by the use of hybrid functionals, which include part of the electron-electron interaction exactly and thereby improve on the weaknesses of semilocal exchange functionals as provided by the local density and generalized gradient approximations. Much better agreement with photoemission data as compared to previous calculations is found and a consistent description of the rutile-type early transition-metal dioxides is achieved. In particular, the results obtained for VO_2 are in line with previous calculations for NbO_2 and MoO_2.