The role of dimers in the metal-insulator transitions in VO$_2$ and Ti$_2$O$_3$

T.C. KOETHE, J. GEGNER, Z. HU, C. SCHÜSSLER-LANGEHEINE, H. ROTH, T. LORENZ, II. Physikalisches Institut, Universität zu Köln, Germany, F. VENTURINI, N.B. BROOKES, ESRF, Grenoble, France, W. REICHELT, Institut für Anorganische Chemie, TU Dresden, Germany, L.H. TJENG, II. Physikalisches Institut, Universität zu Köln, Germany — The nature of the metal-insulator-transition (MIT) in VO$_2$ has been subject of debate for a long time. Recently the scenario of an orbital assisted MIT has been proposed on the basis of the dramatic change of the orbital occupation as observed by soft-X-ray absorption spectroscopy measurements.$^1$ We present the results of our bulk sensitive photoemission study on the MIT in VO$_2$ using high quality single crystals. We observe a huge transfer of spectral weight across the MIT, supporting recent LDA+DMFT cluster calculations.$^2$ To investigate the possible role of dimers herein, we also studied the insulating phase of Ti$_2$O$_3$. Here we clearly observe a double peak structure which can be taken as a characteristic for the presence of dimers.

$^1$M.W. Haverkort et al., PRL 95, 196404 (2005).

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