The curious case of the B-phase VO_2: a bad to worse insulator transition

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Materials in which sudden changes in conductive properties can be induced by external stimuli have multifarious applications. An iconic example is vanadium dioxide, VO_2. Its metal-insulator transition at Tc = 340 K has been rationalized by an accompanying structural transition below which vanadium atoms pair-up into dimers and electronic correlations promote a non-local spin-singlet state. Besides this standard crystal-structure, VO_2 can exist in a panoply of polymorphs. Particularly attractive is the relatively unexplored B-variant: Its resistivity switches by over four orders of magnitude at slightly lower, and therefore, more useful temperatures. Intriguingly, the transition is iso-structural, with dimers present above and below Tc, challenging the scenario for "standard" VO_2. Combining comprehensive experiments with many-body simulations, we reveal[1] that the resistive switching in B-VO_2 is not, in fact, due to a metal-to-insulator transition at all, but to an unconventional transition between a bad and a worse insulator. We argue that, above Tc, the singlet in B-VO_2 is destabilized by a charge-transfer mechanism, despite the structural dimerization. The emergence of incoherent in-gap weight then leads to residual conduction in an otherwise gapped ground-state. Monitoring the Einstein-Podolsky-Rosen-like quantum-entangled singlet state for varying temperatures and across polymorphs, we establish a compendious microscopic picture of the VO_2 system.

References

[1] Banabir Pal, Amar Srivastava, Abhinav Kumar, Sumanta Mukherjee, Indranil Sarkar, Mihaela Gorgoi, Paola Di Pietro, Stefano Lupi, W. Drube, E. Arenholz, J. Chakhalian, A. Perucchi, T. Venkatesan, S. Biermann, J. M. Tomczak, and D. D. Sarma (Unpublished).