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Electronic excitations in Vanadium Dioxide (VO_2) MATTEO GATTI, European Theoretical Spectroscopy Facility (ETSF) and LSI, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France, FABIEN BRUNEVAL, European Theoretical Spectroscopy Facility (ETSF) and ETH Zurich, Dept. Chem. and Appl. Biosciences, CH-6900 Lugano, Switzerland, VALERIO OLEVANO, European Theoretical Spectroscopy Facility (ETSF) and LEPES, CNRS, 25 Avenue des Martyrs, F-38042 Grenoble, France , LUCIA REINING, European Theoretical Spectroscopy Facility (ETSF) and LSI, Ecole Polytechnique, CNRS-CEA/DSM, F-91128 Palaiseau, France — Vanadium dioxide has a metal-insulator transition at $T_C = 340$ K. The role of correlation in this first-order transition has been debated for a long time: is VO_2 a Peierls or a Mott-Hubbard insulator? Despite a good agreement with experimental lattice parameters, DFT-LDA yields a negative gap in the insulating phase and hence is not able to give a good answer to this question. This seeming failure of LDA is discussed and different possible approaches to solve this problem are reviewed: from standard perturbative G_0W_0 to self-consistent GW. Also results concerning other kinds of electronic excitations (in particular: electron energy loss spectra) are presented.

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