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Interplay of oxygen vacancies and electronic correlations in $SrVO_3$[1] STEFFEN BACKES, AARAM J. KIM, Institut für Theoretische Physik, Universität Frankfurt, FRANK LECHERMANN, Institut für Theoretische Physik, Universität Hamburg, HARALD O. JESCHKE, Institut für Theoretische Physik, Universität Frankfurt, MARCELO J. ROZENBERG, Laboratoire de Physique des Solides, Université Paris-Sud, ANDRES F. SANTANDER SYRO, CSNSM, Université Paris-Sud and CNRS/IN2P3, ROSER VALENTI, Institut für Theoretische Physik, Universität Frankfurt — We investigate the role of oxygen vacancies in $SrVO_3$ within LDA+DMFT (density functional theory combined with dynamical mean-field theory). We show that, in addition to the usual t_{2g} lower Hubbard band, oxygen vacancies are responsible for an additional peak around -1 eV of V $3d_{z^2}$ orbital character, which is not present in the bulk system without vacancies. We discuss our results in the light of recent angle-resolved photoemission (ARPES) experiments.

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