## Abstract Submitted for the MAR12 Meeting of The American Physical Society

Implementation of a dynamical cluster approximation within an augmented plane-wave framework HUNPYO LEE, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, KATERYNA FOYEVTSOVA, JOHANNES FERBER, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany, MARKUS AICHHORN, Institute of Theoretical and Computational Physics, TU Graz, Graz, Austria, HARALD O. JESCHKE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany — Even though the local density approximation in combination with dynamical mean field theory (LDA+DMFT) accounts for various and interesting physics such as Mott insulator and enhancement of effective mass for real compounds, the pseudo-gap and spin density wave behaviors are missed due to the absence of spatial correlations. In order to consider the short-range spatial correlations beyond the LDA+DMFT approach for real compounds, we introduce a combination of LDA with a dynamical cluster approximation (LDA+DCA) in the framework of the full-potential linear augmented plane-wave basis and show results for SrVO3. We discuss how to implement the LDA+DCA approach in the WIEN2k density functional theory code and analyze the momentum spectral properties on SrVO3 as a result. We compare our LDA+DCA results with LDA+DMFT as well as with angle-resolved photoemission spectra (ARPES). We find that LDA+DCA results compare better with ARPES than the LDA+DMFT results due to inclusion of spatial correlations.

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