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Application of Projective QMC to LDA+DMFT calculations for LiV_2O_4 RYOTARO ARITA, RIKEN (The Institute of Physical and Chemical Research), KARSTEN HELD, MaxPlanck Institute for Solid State Research, ALEXEY LUKOYANOV, Ural State Technical University-UPI, VLADIMIR ANISIMOV, Institute of Metal Physics, Russian Academy of Science-Ural division — By means of the LDA+DMFT method (the local density approximation combined with the dynamical mean field theory), we investigate the electronic structure of LiV_2O_4, for which various heavy-fermion-like behaviors have been observed experimentally. To obtain the spectral function at $T \to 0$, we employ the projective quantum Monte Carlo method as the solver of the effective impurity problem in DMFT. We show that a sharp peak appears just above the Fermi level at $T \to 0$, which is consistent with the recent photoemission experiment by Shimoyamada *et al.* [Phys. Rev. Lett. **96** 026403 (2006)]

Ryotaro Arita
RIKEN (The Institute of Physical and Chemical Research)

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