Angle-resolved Resonant Inelastic X-ray Scattering in NaV$_2$O$_5$\textsuperscript{1}

GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, IN 47809, T.A. CALLCOTT, Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN — Angle-dependent resonant inelastic x-ray scattering spectrum at the V-$L_3$ edge is analyzed to determine the origin of the V-$dd$ peak in NaV2O5 \cite{1}. Experiment shows that as the incident photon polarization is rotated from the $b$ to $c$ axis, the V-$dd$ peak grows relative to the V-$d$/O-$p$ peak and its energy loss becomes larger \cite{2}. Our first-principles calculations demonstrate that such growth must involve both the unoccupied dxy and dxz/dyz bands. Neither the dxz/dyz nor dxy excitation alone can reproduce the ratio change. For the bc scan, the light first samples the dxy orbital and then the dxz/dyz orbital. Slightly detuning the incident energy away from the resonant edge reveals that the dxy band is slightly lower in energy and much narrower than the dxz/dyz band. The results suggest that our previous analysis of the correlation splitting of the dxy band is valid \cite{3}. \cite{1} G. P. Zhang, T. A. Callcott, G. T. Woods, \textit{et al} Phys. Rev. Lett. \textbf{88}, 077401 (2002); \cite{2} G. P. Zhang \textit{et al}., Phys. Rev. B \textbf{65}, 165107 (2002); \cite{3} G. P. Zhang and T. A. Callcott, Phys. Rev. B \textbf{73}, 125102 (2006).

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