

Abstract Submitted
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Angle-resolved Resonant Inelastic X-ray Scattering in NaV_2O_5 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 NaV_2O_5 [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 [2]. Our first-principles calculations demonstrate that such growth must involve both the unoccupied d_{xy} and d_{xz}/d_{yz} bands. Neither the d_{xz}/d_{yz} nor d_{xy} excitation alone can reproduce the ratio change. For the bc scan, the light first samples the d_{xy} orbital and then the d_{xz}/d_{yz} orbital. Slightly detuning the incident energy away from the resonant edge reveals that the d_{xy} band is slightly lower in energy and much narrower than the d_{xz}/d_{yz} band. The results suggest that our previous analysis of the correlation splitting of the d_{xy} band is valid [3]. [1] G. P. Zhang, T. A. Callcott, G. T. Woods, *et al* Phys. Rev. Lett. **88**, 077401 (2002); [2] G. P. Zhang *et al.*, Phys. Rev. B **65**, 165107 (2002); [3] G. P. Zhang and T. A. Callcott, Phys. Rev. B **73**, 125102 (2006).

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