Zhang *et al.* Reply: We respond briefly to several comments of Duda *et al.* [1]. They base their comments on a cluster model in which crystal field splittings are introduced "by hand" to account for the effect of adjacent atoms and on a qualitative statement of the strengths of transitions without calculating the appropriate matrix elements [1]. Our conclusions are based (1) on band structure calculations which automatically include all crystal field effects and (2) on a model cluster type calculation that accurately includes correlation effects for the weakly hybridized d_{xy} band that spans the Fermi level, but not for the band structure features associated with V/O hybridization [2,3]. The band structure calculations yield projected densities of states of s and p symmetries at each of three oxygen sites, of s, p, and d symmetries at the V site, and transition matrix elements between all states. The calculations show that the Fermi level lies at the center of a narrow band formed by V-d_{xy}/V-d_{xy} interactions while all other d orbitals are strongly hybridized and form broad V-d/O-p bands whose edges lie 1 eV or more away from the Fermi level.

The "crystal field" splittings cited by the commenters refer roughly to the energy differences between the states of d_{xy} and of d_{xz} and d_{yz} symmetry in our calculations. Their claim is that the energy losses observed in resonant x-ray scattering spectroscopy (RIXS) correspond to electron excitations of the type $d_{xy} \rightarrow d^*_{xz} + d^*_{yz}$. We contend the excitations are of type $d_{xy} \rightarrow d_{xy}$ where the excitations are between initial and final states split by the correlation gap.

Our experimental data show that (1) there is a narrow energy loss peak centered at -1.56 eV and a broader peak to lower energy and (2) that the -1.56 eV peak is sharply resonant in energy near the threshold of the V-L3 excitation. (1) requires that there be a narrow density of states (DOS) feature in the final state of the RIXS process located about 1.56 eV above the filled d_{xy} band and (2) requires that there be a narrow feature in the intermediate state of the RIXS process. These features are not observed in the calculated DOS of the d^*_{xz} or d^*_{yz} states. If they are present, they must be due to excitonic states that are not included in the band structure calculations. In contrast, our model calculation for RIXS energy loss to excitation between Hubbard bands show both features of the published data.

The antibonding (i.e., antisymmetric) band formed by the d_{xy} orbitals does produce a narrow DOS feature above the Fermi level. However, the d_{xy} (symmetric) $\rightarrow d^*_{xy}$ (antisymmetric) transition is forbidden in the RIXS process. This may be the source of the statement by the commenters in their first paragraph that the $d_{xy} \rightarrow d^*_{xy}$ transition is forbidden. However, d-d transitions are not forbidden between the correlation split Hubbard bands which are both formed from the bonding (symmetric) orbitals.

The commenters state on qualitative grounds that the "spectral signatures" are weak. The question of course is how weak. The observed -1.56 eV peak in the data is in fact observed to be relatively small and to become more prominent only when resonantly enhanced by the RIXS process. The dispute about the interpretation of our data can best be resolved by calculations of the RIXS processes including realistic calculations of the matrix elements. We are currently undertaking such calculations.

We comment briefly here on several aspects of the Comment. They claim that oxygen atoms in the bridging position on the rungs in NaV_2O_5 are strongly hybridized with the vanadium atoms. Band structure calculations show clearly that these hybridized d bands involve d_{xz} and d_{yz} orbitals and fall far below the Fermi level. The V-d_{xy} "bonding" band at the Fermi level is not hybridized with the bridging O(1) atoms on the ladder rungs. The narrow "antibonding" band formed from these states and lying about 1 eV above the Fermi level does show hybridization with the bridging O(1) atoms. The information obtained at the O-K edge cannot be directly compared with our RIXS spectrum since they probe different states. The transitions leading to their observed energy losses probably involve O-p orbitals that hybridize with the V-d_{xz} and d_{yz} orbitals. If they involve V-d_{xy} orbitals at all, it is probable that the energy loss corresponds to the energy between d_{xy} bonding and antibonding states. The claim of consistency with the values obtained from optical spectra is problematic since optical and RIXS have different selection rules and probe different states.

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