Duda *et al.* Reply: We have reported energy loss features at 0.8 eV, 1.75 eV, 4–5 eV, and 7.0 eV in resonant inelastic x-ray scattering (RIXS) experiments of NiO at the O 1*s* edge [1]. Hüfner *et al.* [2] criticized our interpretation of the two latter excitations by a comparison of the RIXS data with x-ray absorption spectroscopy (XAS) and x-ray emission spectroscopy (XES) data. We show in the following that they are incorrect and that their attempt to determine the excitation energies of RIXS by combining XAS and XES data on an artificial binding energy scale is flawed. This is easily understood from that XAS peak energies are strongly affected by the core hole potential, whereas RIXS peak energies are quite independent of the core hole potential.

(1) We interpreted the strongest excitation at about 7 eV as the charge transfer (CT) excitation from the d^8 ground state to a nonbonding $d^9\underline{L}$ state. Hüfner *et al.* claim that this contradicts with O 1*s* XAS and XES experiments by Schuler *et al.* [3], which seem to suggest that the 7 eV excitation is a CT excitation out of the O 2*p* density of states h_p (at 4.5 eV) into the d^9 state (denoted as d^9L in [2]) at 2.5 eV in the XAS spectrum. They also point out the apparent discrepancy between our value for $\Delta = 3.8$ eV and the excitation energy for the $d^8 \rightarrow d^9\underline{L}$ (7.0 eV). First, when discussing RIXS excitation energies the XAS energy (2.5 eV) for the d^9 state cannot be used because XAS is affected by a core hole potential. Instead, the bremsstrahlungs isochromate (BIS) peak position should be used which is well known to be 4.0 eV [4]. Second, there is no contradiction between using $\Delta = 3.8$ eV and the excitation energy value of $d^8 \rightarrow d^9\underline{L}$. This is because the CT excitation energy of $P3$ is not only determined by Δ but also by the exchange energy J_H associated with the Hund's rule coupling—not included in the commonly used definition of Δ—and a lowering of the ground state energy due to hybridization, δE_G. Therefore, the relevant excitation energy is approximately given by $\Delta + J_H + \delta E_G$ [5], which is equal to 6.6 eV with $J_H = 1.3$ eV and $\delta E_G = 1.5$ eV. In our numerical calculation, the excitation energy of $P3$ is given by 6.3 eV, in good agreement with this estimation.

(2) We have assigned the 4–5 eV peak ($P4$) (denoted as "4.3 eV peak" in [2]) as a $(d^8, d^8) \rightarrow (d^9, d^8\underline{L})$ nonlocal charge transfer process. Hüfner *et al.* claim that the energy of this excitation should be equal to "the sum of the first ionization energy and the first electron affinity energy", which is 5.7 eV instead of 4.3 eV, and that the 4.3 eV peak can be interpreted as "a one Ni ion on site gap transition out of the valence band into the conduction band". Their interpretation is based on the experimental result by Schuler *et al.* [3], which originally shows that the absolute energy difference between the lowest Ni L_3 XAS peak (as well as the lowest O 1*s* XAS peak) and the highest Ni L_α XES peak (as well as the highest O *K* XES shoulder) is about 3.5 eV (not 4.3 eV), corresponding to the Ni 3*d* to 3*d* transition across the Mott-Hubbard gap (called "one Ni ion on site gap" in [2]). However, if we use again the correct value for the d^9 excitation energy (4.0 eV), the relevant excitation energy becomes 5.5 eV, which is very close to the 5.7 eV. The Ni 3*d*-3*d* gap of 3.5 eV appears only as an unphysical artifact produced by the combination of XAS and XES and does not really exist as such in NiO. Instead, the origin of the RIXS peak at 4–5 eV is essentially the same as that of the 5.7 eV insulating "gap" (the real gap being 4.3 eV) obtained as the energy difference of the lowest BIS peak and the highest photoemission spectroscopy (PES) peak. We consider that the difference between the RIXS excitation energy 4–5 eV and the energy 5.7 eV is a consequence of transfer of oscillator strength in RIXS due to the interaction, absent in BIS or PES alone, between d^9 and $d^8\underline{L}$ states.

(3) Finally, Hüfner *et al.* suggested a possibility that the 1.75 eV peak originates from the crystal field (*d*-*d*) transitions instead of the double singlet creation (DSC). We cannot completely exclude this possibility, because our model used in [1] describes DSC but cannot describe crystal field transitions and intra-atomic multiplet coupling effects. Although confirmation by improved RIXS experiments is desirable, positive evidence is given by the matching polarization dependence of the DSC peak between a preliminary RIXS spectrum calculation of ours including crystal field transitions (without multiplet coupling) and experiment.

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[1] L.-C. Duda, T. Schmitt, M. Magnuson, J. Forsberg, A. Olsson, J. Nordgren, K. Okada, and A. Kotani, Phys. Rev. Lett. **96**, 067402 (2006).

[2] S. Hüfner, S. Schmidt, and F. Müller, preceding Comment, Phys. Rev. Lett. **97**, 269701 (2006).

[3] T. M. Schuler, D. L. Ederer, S. Itza-Ortiz, G. T. Woods, T. A. Callcott, and J. C. Woicik, Phys. Rev. B **71**, 115113 (2005).

[4] G. A. Sawatzky and J. Allen, Phys. Rev. Lett. **53**, 2339 (1984); S. Hüfner, Adv. Phys. **43**, 183 (1994).

[5] See, for a similar argument, A. Fujimori, A. E. Bocquet, T. Saitoh, and T. Mizokawa, J. Electron Spectrosc. Relat. Phenom. **62**, 141 (1993).