Williams, Kübler, and Terakura Respond: Professor Merlin states the following:

(a) That his resonant-Raman measurements indicate that the 4-eV optical-absorption edge in NiO is due to transitions between different atoms. We completely agree.

(b) That there are only two interatomic transitions that are likely to produce the absorption edge: from oxygen to nickel, or from one nickel to a second nickel. (Let us call these two possibilities the one-nickel and two-nickel pictures.) We agree.

(c) That the resonant-Raman measurements do "not bear on the question of the presence of empty *d* states close to the top of the valence band." We agree, but see below.

(d) That all the evidence together supports the two-nickel interpretation. We disagree.

With regard to point "c", while we agree that the resonant-Raman measurements cannot, by themselves, discriminate between the one- and two-nickel pictures (because both pictures are based on interatomic transitions), it is also true that these measurements together with the recent high-resolution photoemission measurements of McKay and Henrich and our calculations offer an attractively simple and consistent interpretation of the absorption edge. This interpretation (one-nickel) ascribes the absorption edge to transitions out of the oxygen *p* bands, which the new photoemission clearly shows to be more than 2 eV below the top of the valence band, into empty *d* states necessarily close to the top of the valence band.

In his last paragraph, Professor Merlin rejects the one-nickel picture, but without explicitly saying why. What he does say suggests that he and we interpret differently the d^8L labeling given the states near the top of the valence band by Fujimori and Minami, on the basis of configuration-interaction (CI) calculations. In our view, the energy-band and the CI calculations are fundamentally consistent, the latter providing a complementary framework within which spectral weight can be apportioned between fully screened excitations lying close to the Fermi level (valence band) and less screened excitations lying volts below the valence band (satellite). The band calculations describe only fully screened excitations, and they are not explicit as to the composition of the exchange-correlation screening hole. In other words, the "L" in the label d^8L refers neither to the symmetry of the state nor to its spatial position, but to the origin of its electronic polarization cloud.

The measurements that deal most directly with the one- versus two-nickel question are those of Blazey,[1] who studied optical absorption in MgO in which a small fraction of the Mg ions were replaced by Ni ions. The Ni concentration was so low that there was effectively no second Ni. Therefore, to the extent that the absorption in MgO:Ni is similar to that in NiO, the one-nickel picture is supported. The absorption in MgO:Ni is similar to that in NiO, but the edge occurs at 6 rather than 4 eV. We have analyzed this 2-eV difference using super-cell energy-band calculations. (The impurity system was approximated by the compound Mg_7NiO_8.) We find that the *p*-to-*d* energy separation depends extremely sensitively on the Ni-O distance, and that the observed *p*-to-*d* energy separation results when the octahedron of oxygen anions surrounding the Ni ion is allowed to relax to the size it has in NiO. (The lattice constant of MgO is 1% greater than that of NiO.) So, we believe the MgO:Ni measurements, in conjunction with our calculations, both support the one-nickel picture, and indicate the importance of polaronic screening. (See below.)

With regard to the weight of the evidence presently available (point d), in our view, most measurements support the one-nickel picture. In particular, scanning tunneling spectroscopy measurements[2] reveal a high density of charge-carrying excitations less than an electronvolt above the Fermi level of oxidized portions of a Ni surface. Furthermore, the optical matrix element should be far stronger for transitions between chemically bonded atoms (one-nickel) than for those between chemically independent Ni atoms (two-nickel). The factor of 5 increase in the Néel temperature across the series MnO, FeO, CoO, and NiO also suggests that the gap within the *d* states decreases towards zero. Multiple charge states are observed for many transition-metal impurities in semiconductors, indicating the effectiveness of local screening in reducing the effective U.[3,4] The empty *d* states in NiO are likely to represent the strong-coupling regime of the Haldane-Anderson theory[3] of multiple charge states, if the theory is generalized to include polaronic screening. (Recall that these states are the antibonding partners of the covalent portion of the nickel-oxygen bond.) Even the one experiment that is seemingly inconsistent with the one-nickel picture, the inverse-photoemission measurements of Sawatzky and Allen, becomes consistent, if we argue that the speed of this high-energy experiment does not permit polaronic screening (the Franck-Condon principle).

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