Brühwiler *et al.* Reply: Meinders, Tjeng, and Sawatzky [1] make a valid criticism of the model dependence of our conclusions [2] related to the question of the normal state resistivity of the alkali fullerides. However, their Comment is based on a simple form of the extended Mott-Hubbard model and is applied to a one-dimensional (1D) system only. The extrapolation of their results to 3D is not transparent and yet is the basis for the strong conclusions in their Comment. We will discuss this and attempt to clarify further the nature of the intermolecular core exciton [2].

We determined [2] a lower limit on V which strongly supports the theoretical result of Antropov, Gunnarsson, and Jepsen [3]. This does not seem to be in question. The extrapolation of the fact that $(U - V)/W \approx 1$ to the notion that the correlation-induced conductivity gap may be quenched was put forth there [3] and utilized by us, consistent with accepted understanding as expressed by workers in the field of 1D conductors [4] and 3D covalent materials like diamond and silicon [5]. Thus the preceding Comment is the first published work to our knowledge to indicate that for 3D systems there is no effective reduction of U by V with respect to electronic transport properties.

A key aspect of their Comment is the strength of the conclusions. That level of confidence can only be justified at present within the limits of the 1D model they use. In any case, it cannot be ruled out that $U - V$ is the relevant effective on-site correlation to use in considering certain properties. Thus, it is important to have calculations on 3D systems in order to fully understand, e.g., why single-crystal K_3C_{60} does not appear to be a Mott-Hubbard insulator [6].

Meinders, Tjeng, and Sawatzky further state that the threshold for optical transitions to charge-transfer excitons is $U - V$, which "may not be inconsistent" with our interpretation. We would like to clarify our measurements in light of this statement. Two important quantities we derived [2] were the intrasite correlation between a core hole and valence electron ($U_c = 2.2 \pm 0.3$ eV), and a lower limit on V, $V_{\min} = 0.9 \pm 0.4$ eV. Since the threshold we obtained for hopping was $U_c - V_{\min}$ above the first excitation energy, it suggests that that transition [denoted (b) [2]] may actually be directly to the intermolecular exciton. This can be contrasted with our description of (b) as an intramolecular exciton on the isolated molecule [7], which after excitation in the solid decays both by the direct annihilation of the C 1s hole and by hopping to the nearest neighbor to create the intermolecular exciton, i.e., effectively a two-step process. Hence, in our interpretation there is a resonance between the on-site excitation, which for solid C_{60} spectroscopically resembles that for the isolated molecule and the intermolecular exciton. The greater broadening in the case of the solid for transitions (b) and (c) supports our interpretation semiquantitatively [2]. Furthermore, from the experimental intensities in our Fig. 3 [2], there is at least 50% probability for excitation to the same intramolecular state (b) in the solid. The C 1s absorption intensity to a high accuracy reflects the weight of the single-particle final state(s) on the atomic site probed. Hence, to explain the other 50% in terms of transitions directly to the intermolecular exciton, i.e., to unoccupied orbitals on a neighboring molecule, would require that those orbitals had a weight on the probe atom comparable to orbitals on the same molecule with that atom. Other considerations aside, this would lead to a radical restructuring of the electronic structure, and therefore absorption spectrum, which is not observed [2,8].

Thus, only the finite lifetime of the C 1s hole gives one the possibility to measure the hopping strength, and there appears to be no essential improvement on the picture we put forth [2] developing from the alternative point of view [1]. Given this, the intermolecular state would nevertheless be closely degenerate with (b), since we expect a hopping transition to the delocalized state on the time scale of 6 fs [2]. For a final state at lower energy, such hopping would require accompanying electronic excitations to satisfy energy conservation, which one would expect would be disallowed because of the intramolecular bandgap.

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[1] M. B. J. Meinders, L. H. Tjeng, and G. A. Sawatzky, preceding Comment, Phys. Rev. Lett. **73**, 2937 (1994).
[2] P. A. Brühwiler *et al.*, Phys. Rev. Lett. **71**, 3721 (1993).
[3] V. P. Antropov, O. Gunnarsson, and O. Jepsen, Phys. Rev. B **46**, 13 647 (1992).
[4] D. Baeriswyl, in *Theoretical Aspects of Band Structures and Electronic Properties of Pseudo-One-Dimensional Solids*, edited by H. Kamimura (D. Reidel, Dordrecht, 1985), p. 1, who makes use of the work of S. Mazumdar and A. N. Bloch, Phys. Rev. Lett. **50**, 207 (1983).
[5] P. Fulde and G. Stollhoff, J. Phys. (Paris) **50**, 2659 (1989).
[6] X.-D. Xiang *et al.*, Science **256**, 1190 (1992).
[7] B. Wästberg *et al.*, Phys. Rev. B **50**, 13 031 (1994).
[8] However, there should be a finite, but low, probability for direct excitation given by the strength of the mixing between on- and off-site excitons.

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