MICHAEL SCHLÜTER: The late researcher found electron-phonon interactions are responsible for the superconductivity of $A_3C_{60}$.

PHYSICAL CHEMISTRY

Editor's Note: On Nov. 18, 1992, AT&T Bell Laboratories physicist Michael Schlüter passed away. He provided the following information to The Scientist just prior to his death at age 47.


Michael Schlüter (AT&T Bell Laboratories, Murray Hill, N.J.): "The electronic structure of fcc (face-centered cubic) alkali intercalated $A_3C_{60}$ (where $A = K, Rb$ or $Cs$) is studied using the density functional (LDA) approach and a semi-empirical tight binding scheme fit to the results. The picture that emerges is one of tightly bound $C_{60}$ molecules, weakly held together by narrow, almost dispersionless bands. These bands are part of a manifold, derived from a $l = 5$ set of states. The vibrational states of $A_3C_{60}$ are studied in a variety of models, reaching from simple Keating-type and bond charge-type to frozen phonon LDA-type descriptions. From this, a consistent picture of vibronic states emerges, in accordance with a variety of experiments such as Raman and infrared and neutron scattering.

"The interactions between electrons and phonons are calculated and found to be dominated by particular on-ball Jahn-Teller-type vibrations. We propose that the superconductivity found in $A_3C_{60}$ materials arises from these interactions, optimally enhanced by the unique molecular nature of these materials. In particular, a real-space 'factorization' of two different energy scales determines the coupling constant $l = NV$. The electron scattering $V$ is dominated by the large intra-ball p-electron energy scale via the coupling to the Jahn-Teller-type modes. The density of states $N$, on the other hand, is controlled by the weak inter-ball hopping energy scale. This factorization leads to a number of remarkable consequences, such as the scaling of $T_c$ with pressure or lattice spacing, a vanishing alkali isotope effect, a strong carbon isotope effect, strong changes with intercalation in Raman and Neutron spectra, and a simple phase diagram.

The qualitative difference between fullerite and intercalated graphite, with much lower $T_c$ values, can be explained on simple geometric grounds. Finally, the general picture can be used as a basis for speculations about new, potentially high $T_c$ molecular superconductors."