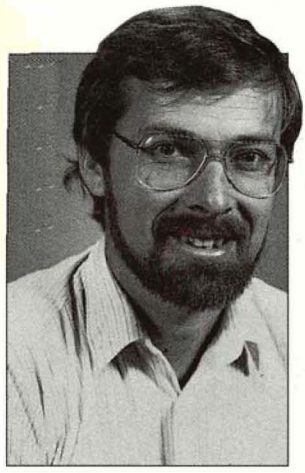
Hot Papers



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.*

M. Schlüter, M. Lannoo, M. Needels, G.A. Baraff, D. Tománek, "Electron-phonon coupling and superconductivity in alkali-intercalated C_{60} solid," *Physical Review Letters*, 68:526-9, 1992.

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."