Surface bands and electron-phonon interactions in field-effect-doped fullerenes

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We have carried out density functional calculations using the SIESTA code [1] to determine the nature of the electron or hole states in field-effect-doped C_{60}, as well as tight-binding and SIESTA calculations of the electron-phonon interactions. The original motivation was the claims of hole-doping and superconductivity at high temperatures, which has now been discredited [2]. Even though the urgency is now missing, the calculations still stand as predictions of what will happen if high fields and high-quality interfaces can be produced in the future. The primary conclusions are: 1) the carriers are confined by the field to the interface in an extremely thin layer of one molecule, so that they are effectively two-dimensional; 2) the states are significantly distorted from bulk-like states due to the high field; 3) the C_{60} molecules are stable even with high doping and fields; and 4) states near the Fermi energy are greatly affected by orientation, so that we expect large effects of disorder and electron-electron interactions.

Electron-phonon interactions were investigated in a series of calculations with extensive use of tight-binding for simplicity, but with checks using SIESTA. The main conclusions are: 1) the coupling for holes is smaller than for electrons; 2) this tends to compensate for the fact that the density of states is higher for holes; and 3) there is an enhancement of the electron-phonon interactions caused to lowering of symmetry. This last conclusion is the most significant as a possible way to enhance superconductivity. The high field effectively lowers the symmetry, allowing different phonon to participate and increasing the overall electron-phonon interaction.

[1] D. Sanchez-Portal, P. Ordejon, E. Artacho, and J. M. Soler, Int. J. Quant. Chem. 65, 453 (1999).
[2] See, for example, the news article by Robert F. Service in Science; 298: 30-31, October 4, 2002.