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 \cite{1} to determine the nature of the
electron or hole states in field-effect-doped C\textsubscript{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 \cite{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\textsubscript{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.

\cite{1} D. Sanchez-Portal, P. Ordejon, E. Artacho, and J. M.
\cite{2} See, for example, the news article by Robert F.
Service in Science; 298: 30-31, October 4, 2002.