

Tunneling Current from Surface States

SEMITIP presently does *not* have the capability of computing current arising directly from surface states. This is a reasonable limitation for the case of *extrinsic* surface states, i.e. ones that arise from defects, etc., that can well be located relatively far from the tunneling tip and thus not contribute directly to the current (they will still contribute indirectly, through their effect on the surface charge, but their direct effects in producing current will be negligible so long as their wavefunctions do not overlap the tunneling area). For the case of *intrinsic* surface states, i.e. ones that exist in every unit cell of the surface this limitation is a severe (and unphysical) approximation. Thus, the SEMITIP package cannot be used in its present form to obtain a realistic estimate of the direct role of intrinsic surface states in affecting the tunnel current.

In the input parameters of the FORT.9 file, two sets of parameters for surface states can, by default, be input. In some instances within the SEMITIP documentation these are associated with intrinsic and extrinsic surface states. The band bending results produced by SEMITIP can thusly account for both intrinsic and extrinsic states, but again, in terms of tunnel current the direct effects of neither intrinsic nor extrinsic states are included.