# Schottky Barrier project

# 2021

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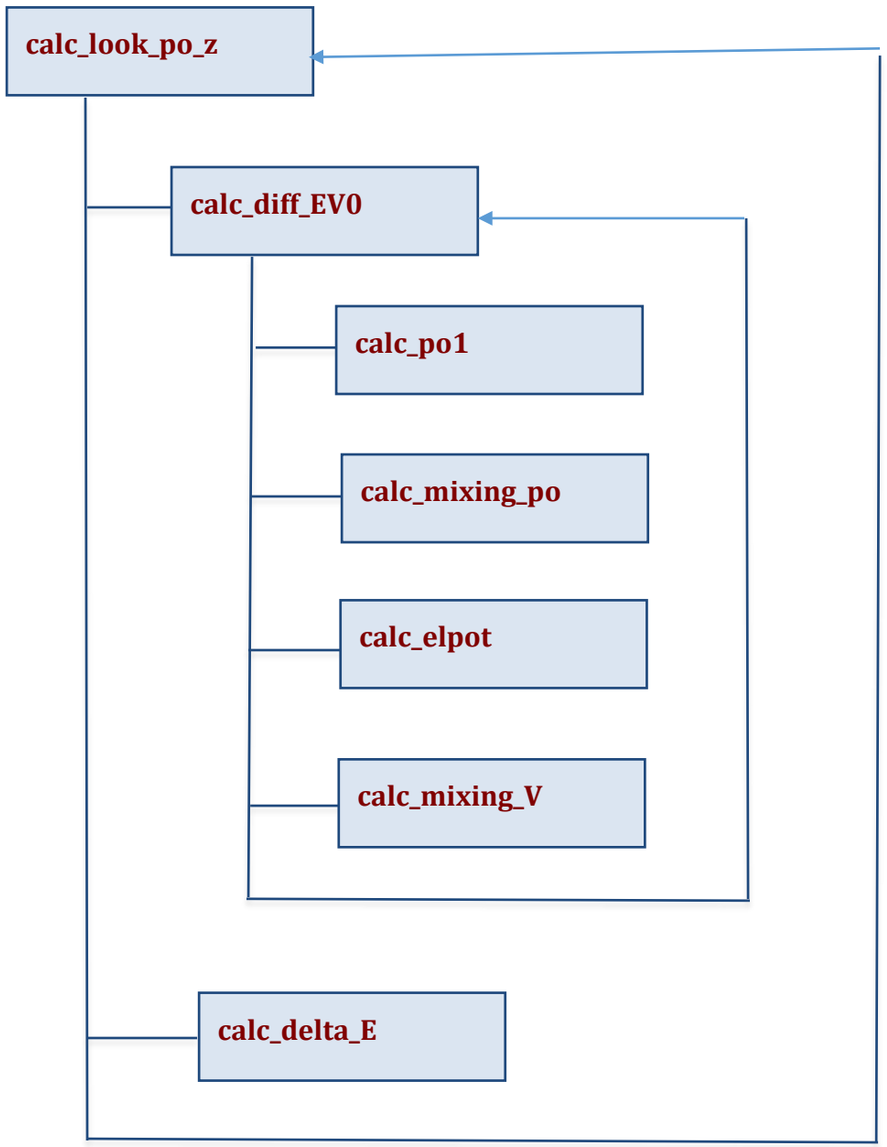
2021

## The structure of SB program

**Schottky_barrier.f90**

- **Parameters.f90** — Set initial parameters, read data from files, allocate arrays, calculate *z*-mesh Zz(Nz), calculate initial approximation for density (po1(Nz)) and potential (V_el1(Nz)) on *z*-mesh
- **Spline_functions.f90** — Extrapolate functions from data points by third order splines (in order to 1) accurately integrate, 2) separate calculation of potential from charge density)
- **Schottky.f90** — Module Schottky, calculate charge densities and Schottky potential (integration)
- **Plot.f90** — Calculate charge densities and potential on *z*-mesh points, mixing with previous iteration and do SCF, write data files

SCF cycle (in module Plot.f90)




Calculate charge density ρ(z) and potential V(z) self-consistently connected

SCF cycle. Initial approximation to ρ(z) and V(z) are formulas (20) and (22)

Calculate ρ(z) using formulas (12) – (16)

Mixing old and new ρ(z) for next iteration

Calculate V(z) using formulas (8) and (10)

Mixing old and new V(z) for next iteration

Calculate ΔE using formula (18)

Repeat SCF cycle until ρ(z) calculated from V(z) will correspond to the V(z) calculated from ρ(z)

Additional modules:

QSL3D.f – subroutine for accurate integration of oscillating function

Parallel.f90 – MPI commands for parallelization over $z$-mesh points

# Input data files:

1 DOS of the bulk SC (dos_bulk_.dat)

2 PDOS of interfacial layer (3d layer - kpdos_int_3.dat, 4th layer - kpdos_int_4.dat, and surface layer - DOS0.dat)

3 CBS data (a set of data files from CBS calculation bands.Si.im1,…)

4 k-mesh data (k_mesh.dat)

5 Polarization data (polarization.dat)

# Prepare calculations:

1 DOS of bulk semiconductor

2 k-separated PDOS for interface calculations for NxNx1 k-mesh

3 CBS calculation for k-mesh corresponding to interface calculation

# Compile the program:

> ./compile_mpi.sh

# To run the program:

```
> schottky 300. 1.35 0. > output
            T    E_F  gate
```

# The calculated results:

1 data file for densities po_.dat (`in the format of z, poh, poe, poMIGS, po`)

2 data file for potential elpot_.dat (in the format of z, V_el, E_field)

3 output file contains all Schottky barrier parameters