Schottky Barrier in QCAD

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June 1, 2015

Potential BC at Schottky Contact

The empirical expressions[1]-[4] for electric potential at Schottky contacts, when solving the Thomas-Fermi Poisson equation in QCAD, are given by

$$\phi_{BC}^{SB} = V_a - \frac{1}{q}\left(q\phi_{Bn} + \chi_{sc} - q\phi_{ref}\right)$$ → for Schottky contact on n-type semiconductor, in unit of Volts

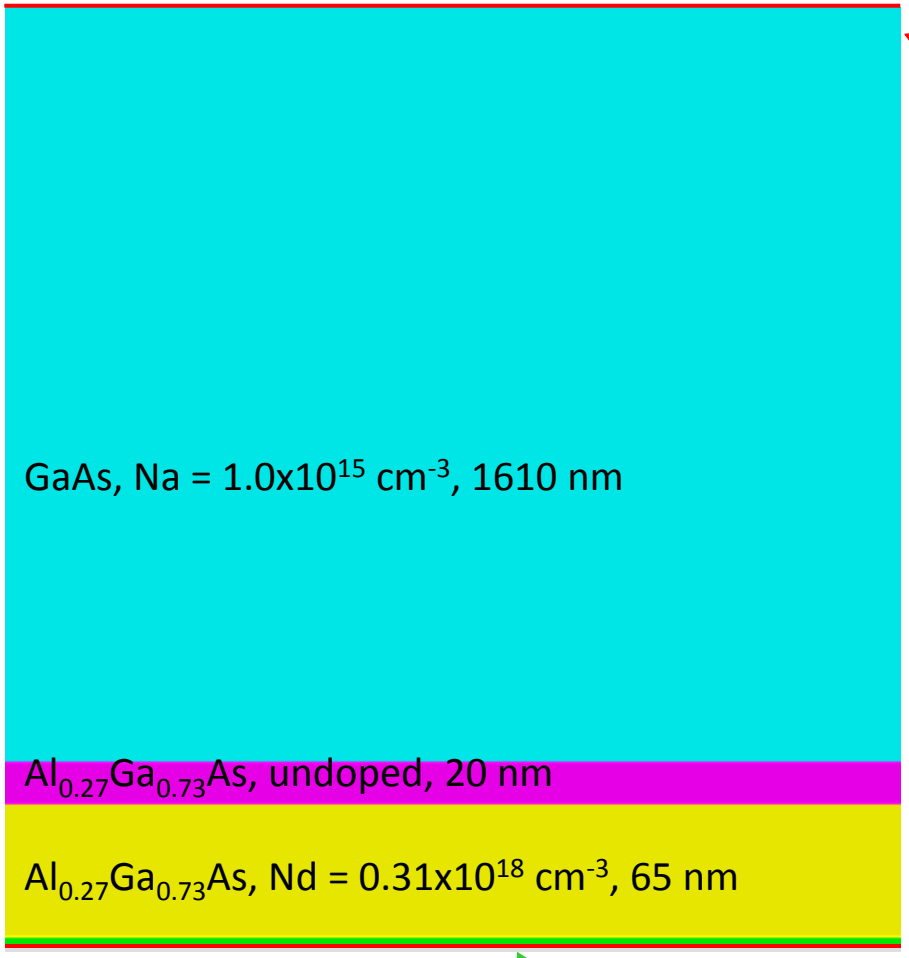
- V_a: applied voltage
- $q\phi_{Bn}$: Schottky barrier height on n-type semiconductor, equal to Ec - Ef > 0
- χ_{sc}: Electron affinity of the n-type semiconductor
- $q\phi_{ref}$: Constant shift between vacuum potential and electric potential

$$\phi_{BC}^{SB} = V_a - \frac{1}{q}\left(-q\phi_{Bp} + \chi_{sc} + E_{g,sc} - q\phi_{ref}\right)$$ → for Schottky contact on p-type semiconductor

- $q\phi_{Bp}$: Schottky barrier height on p-type semiconductor, equal to Ef – Ev > 0
- $E_{g,sc}$: Band gap of the semiconductor

[1] S. M. Sze and Kwok K. Ng, Chapter 3 of *Physics of Semiconductor Devices,* Third Edition (2007).
[2] Raymond T. Tung, Appl. Phys. Rev. **1**, 011304 (2014).
[3] L. X. Zhang et al., Phys. Rev. B **69**, 245301 (2004).
[4] M. Stopa, Phys. Rev. B 54, 13767 (1996).

GaAs/AlGaAs Stack



Stack comes from L. X. Zhang et al., Phys. Rev. B **69**, 245301 (2004).

Contact Specification in QCAD

(1) Both contacts are Ohmic

```
<ParameterList name="Dirichlet BCs">
    <Parameter name="DBC on NS gaaspsub for DOF Phi" type="double" value="0.0" />
    <Parameter name="DBC on NS nschottkygate for DOF Phi" type="double" value="0.0" />
</ParameterList>
```

(2) nschottkygate is Schottky, while gaaspsub is Ohmic

The “Dirichlet BCs” section remains the same

```
<ParameterList name="Schottky Barrier">
   <Parameter name="Schottky Barrier Height for NS nschottkygate" type="double" value="0.8" />
</ParameterList>
```

(3) Both contacts are Schottky

The “Dirichlet BCs” section remains the same

```
<ParameterList name="Schottky Barrier">
    <Parameter name="Schottky Barrier Height for NS nschottkygate" type="double" value="0.8" />
    <Parameter name="Schottky Barrier Height for NS gaaspsub" type="double" value="0.6" />
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```
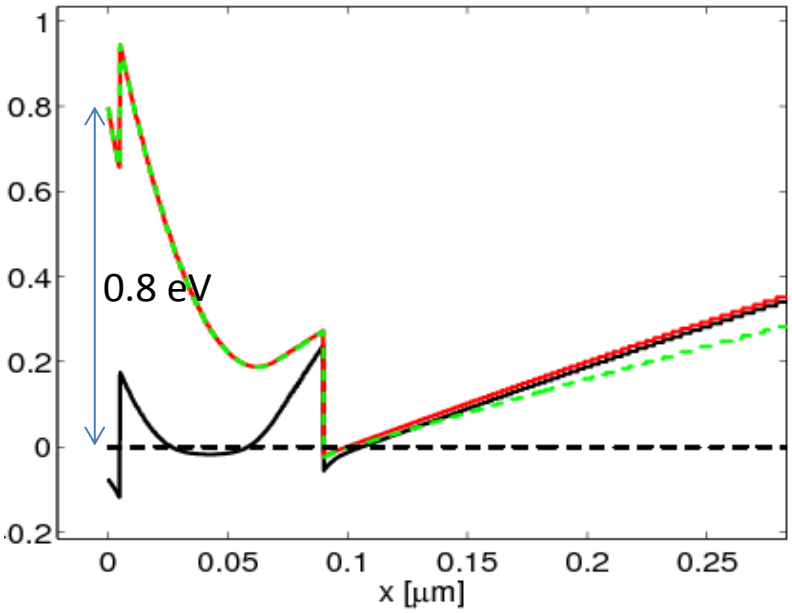
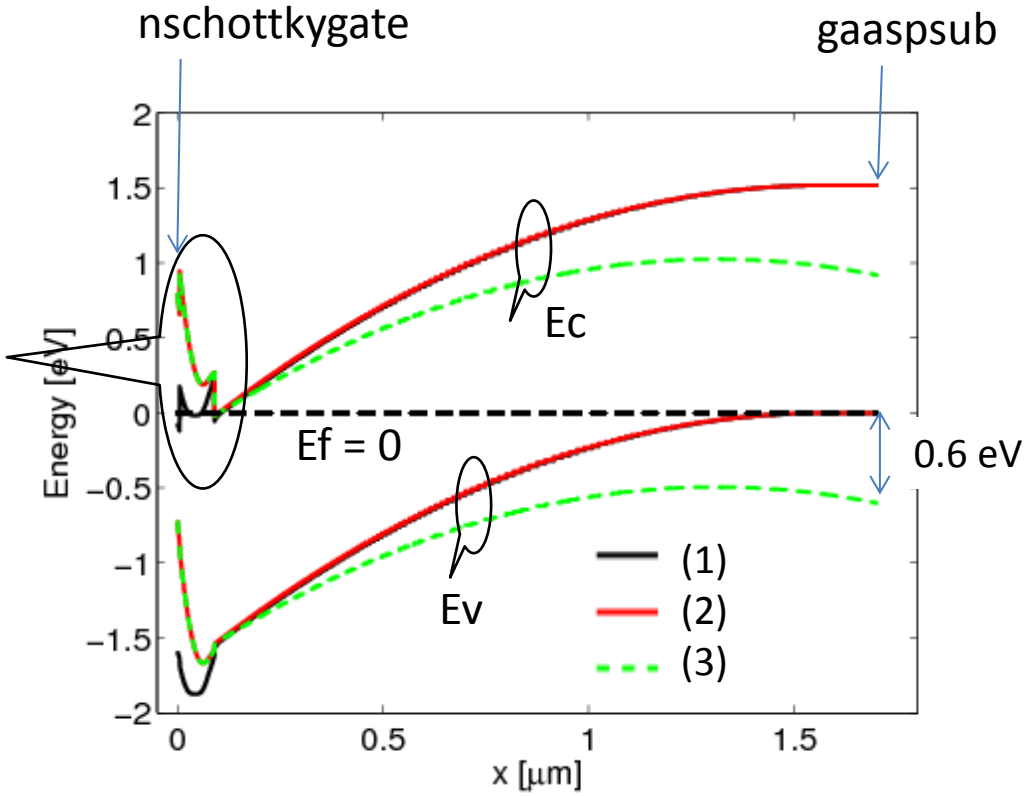

Material properties for GaAs and Al0.27Ga0.73As are added to material_gaas.xml.

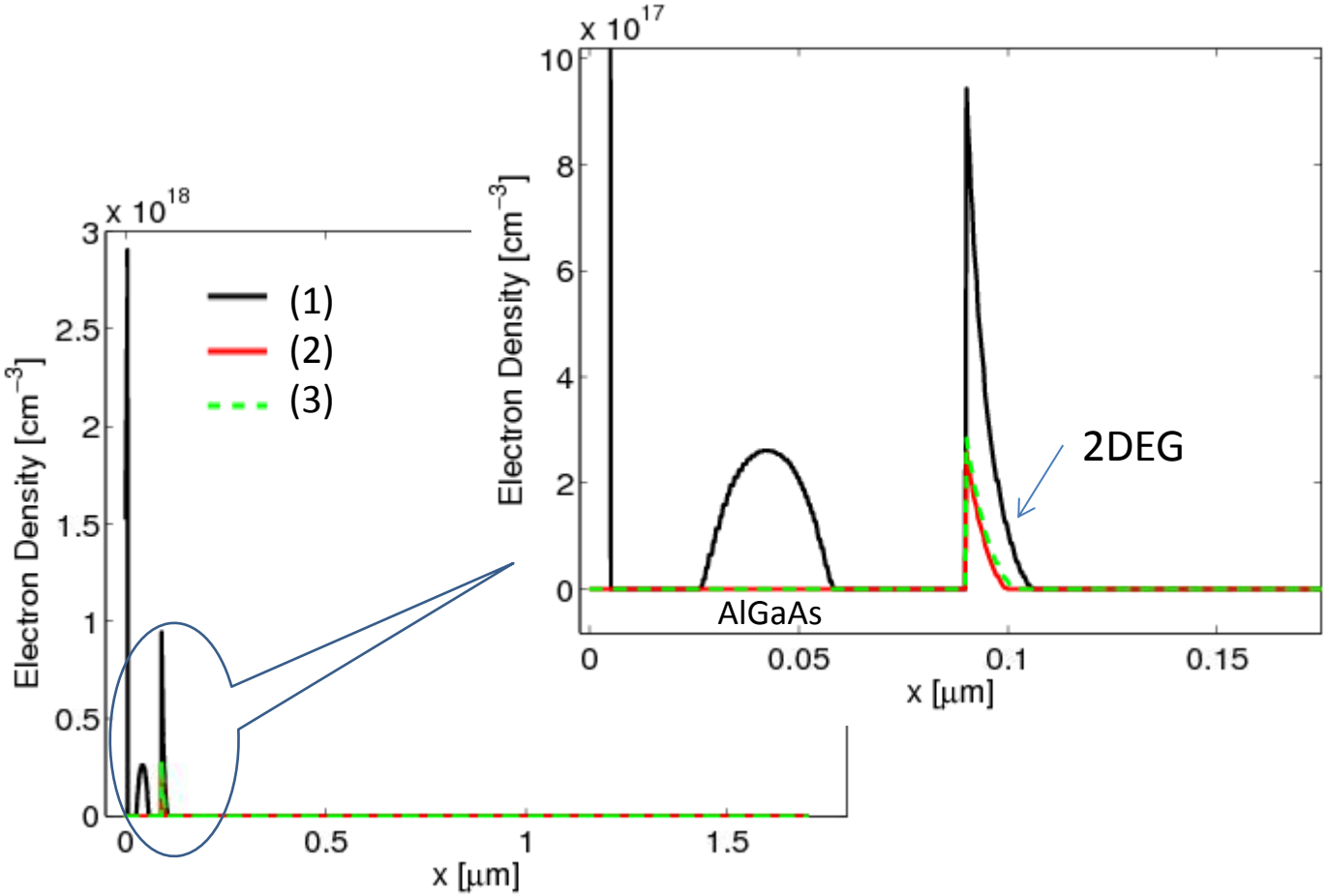
Energy Band at Equilibrium





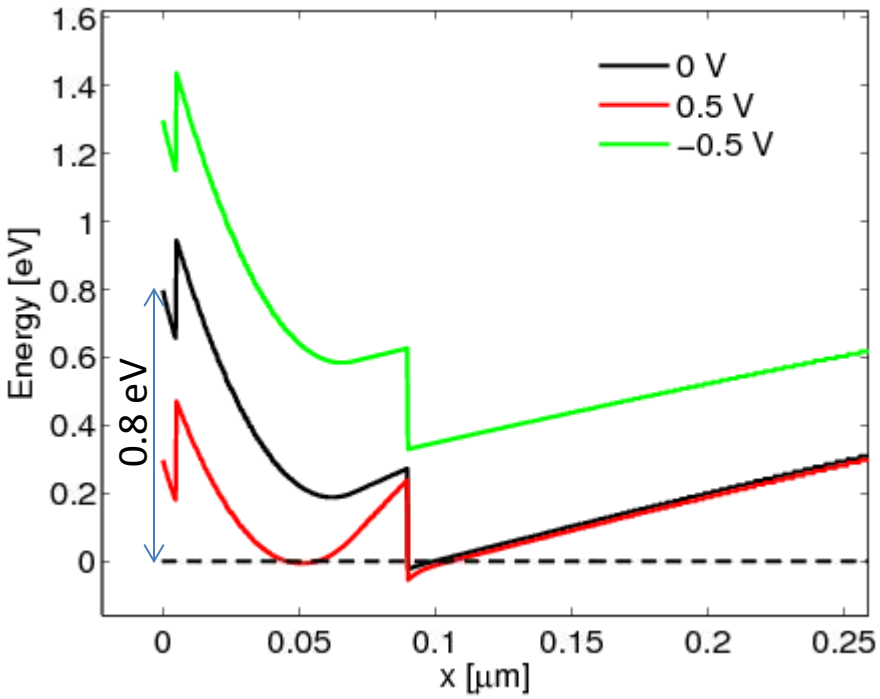
- Barrier height for Schottky contact on n-type semiconductor refers to the difference between Ec and Ef and is positive
- Barrier height for Schottky contact on p-type semiconductor refers to the difference between Ef and Ev and is positive
- Flat band at the Ohmic gaaspsub contact implies good Ohmic
- No flat band for the Ohmic nschottkygate implies that Ohmic assumption is not good

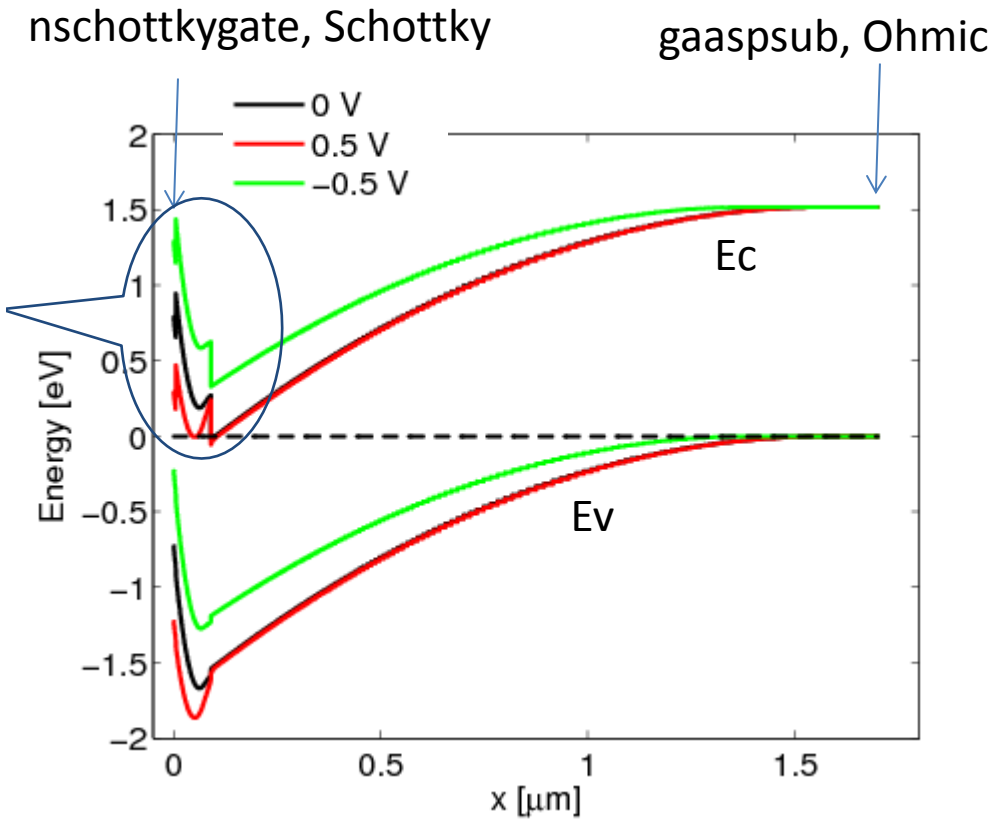
Electron Density at Equilibrium



Electron accumulation in the AlGaAs layer when assuming Ohmic condition for the nschottky contact.

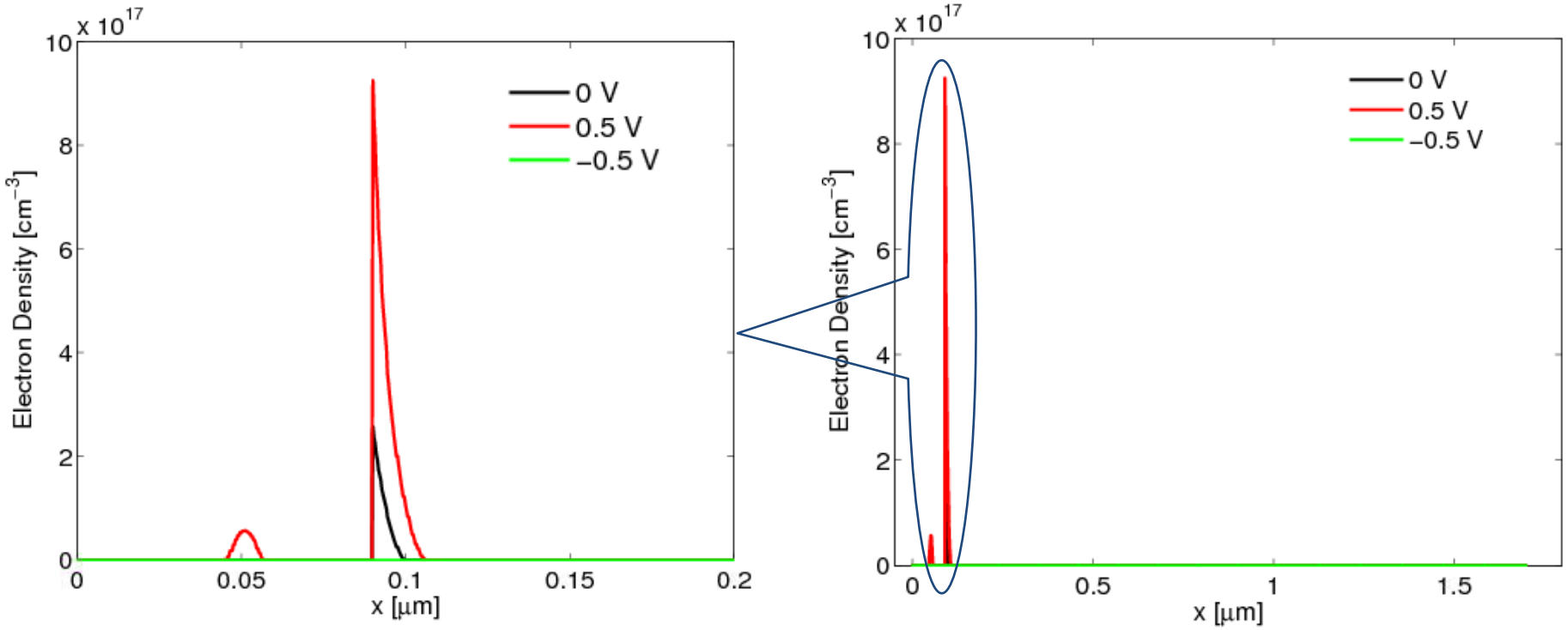
Energy Band Under Bias





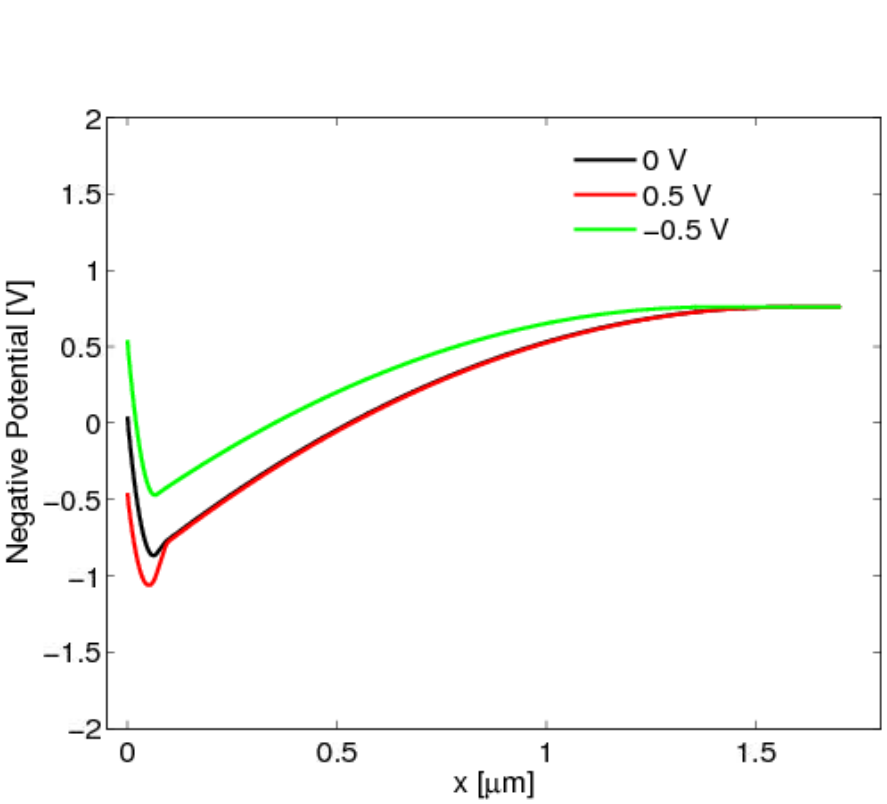
- nschottkygate is a Schottky contact with barrier height of 0.8 eV.
- Positive voltage at nschottky lowers the conduction band
- Negative voltage at nschottky raises the conduction band

Electron Density Under Bias

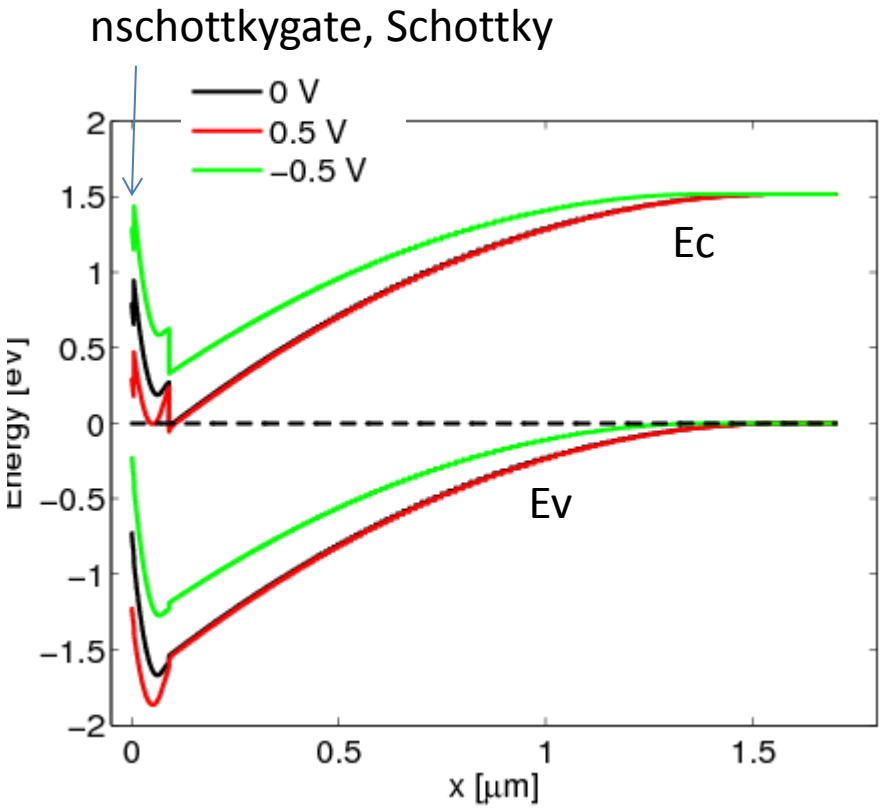


- 2DEG density increases when 0.5 V is applied to nschottkygate
- 2DEG disappears when -0.5 V is applied to nschottkygate

Negative Potential Under Bias



nschottkygate, Schottky



- Conduction bands show quite different profiles from those of the negative potentials, hence one needs to be careful about which quantity to use for further analysis.
- They are related by $-q(\phi - \phi_{ref}) = E_0 = E_C + \chi$ [X. Gao et. al, JAP 114, 164302 (2013)]

potential — conduction band — electron affinity