Overview of quantum potential model implemented into SiLENSe 5.0

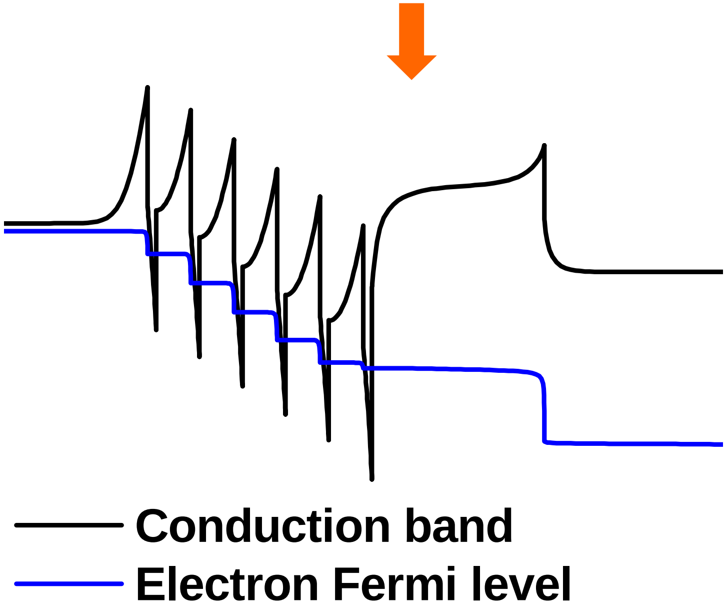
STR 2011

Motivation

For MQW structures, conventional drift-diffusion model predicts a stair-like conduction band profile with a considerable drop of the Fermi level in the spikes of barriers surrounding QWs. This results in a severe over-estimation of the LED turn-on and operation voltages. For InGaN/GaN MQWs, the problem becomes more pronounced with increase of indium content because of both higher band offsets and higher piezoelectric charges at the QW interfaces.

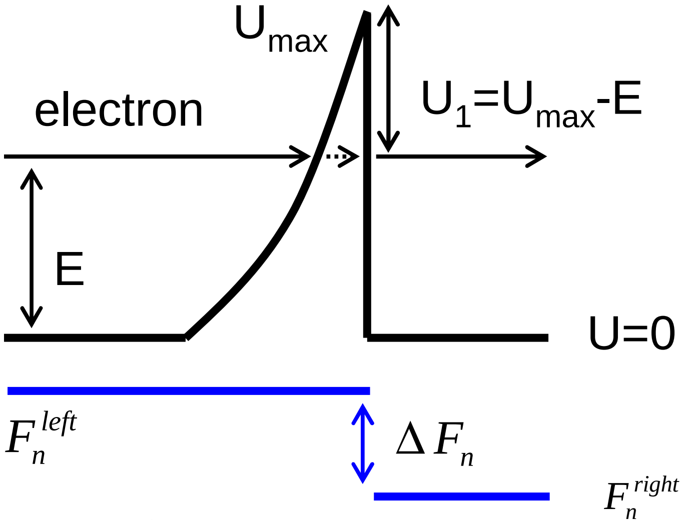
Transport mechanisms beyond drift-diffusion that can contribute to the enhanced carrier transport

- ✓ Tunneling through the barriers
- ✓ Ballistic transport
- ✓ Dislocation-mediated conductivity
- ✓ …



Quantum Effect 1:
Thermal assisted tunneling

Thermal assisted tunneling seems to be the dominant mechanism of the carrier transport in MQWs with high potential barriers originated from both high band offsets and built-in polarization charges



Transmission coefficient

$$D = \exp\left(-\frac{2}{\hbar}\int |\,p(z)\,|\,dz\right), \quad |\,p(z)\,| = \sqrt{2m\big(U(z)-E\big)}$$

Electron flux →

$$J_{\rightarrow} = \frac{mkT}{2\pi^2\hbar^3}\cdot\exp\left(\frac{F_n^{left}}{kT}\right)\cdot\int_0^{\infty} dE\cdot\exp\left(-\frac{E}{kT}\right)\cdot D(E)$$

Electron flux ←

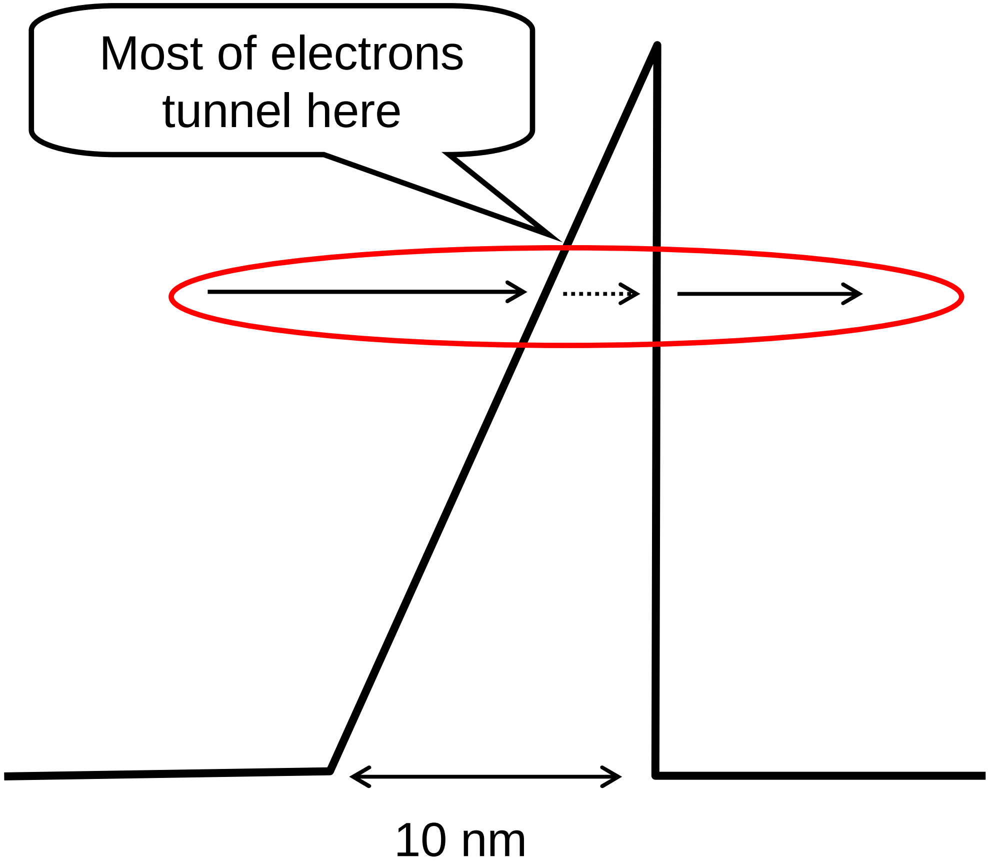
$$J_{\leftarrow} = \frac{mkT}{2\pi^2\hbar^3}\cdot\exp\left(\frac{F_n^{right}}{kT}\right)\cdot\int_0^{\infty} dE\cdot\exp\left(-\frac{E}{kT}\right)\cdot D(E)$$

Total electron flux

$$\boxed{J = J_{\rightarrow} - J_{\leftarrow} = J_{\rightarrow}\left[1-\exp\left(\frac{\Delta F_n}{kT}\right)\right]}$$

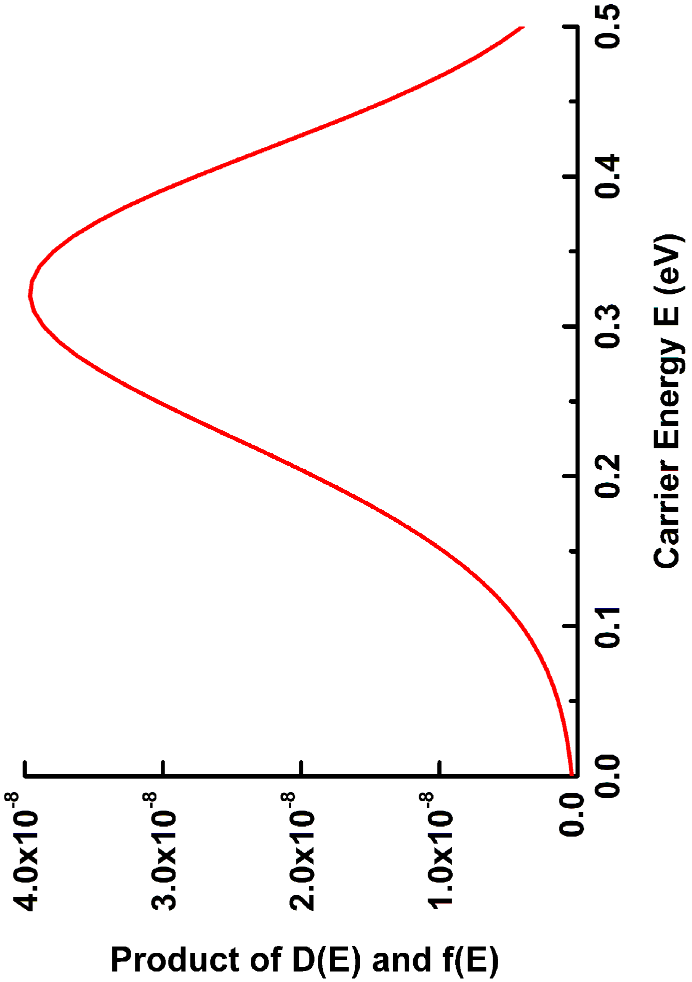
Quantum Effect 1:
Thermal assisted tunneling

Analytical result for a triangular barrier



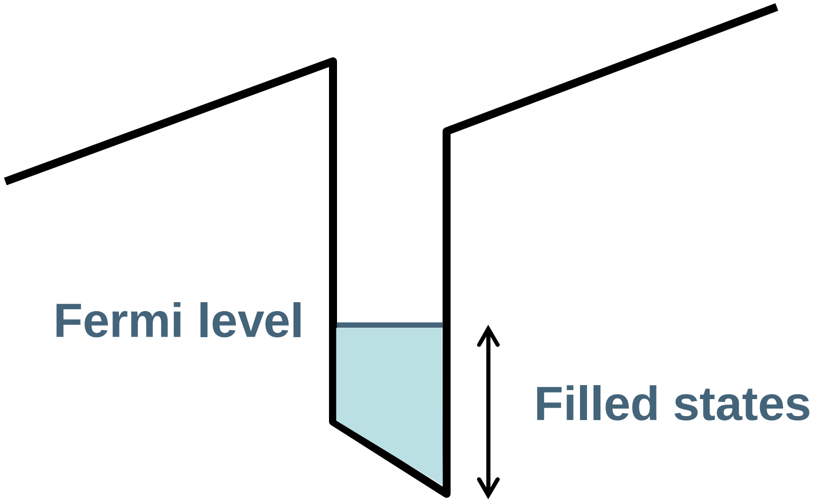
Most of electrons tunnel here

10 nm

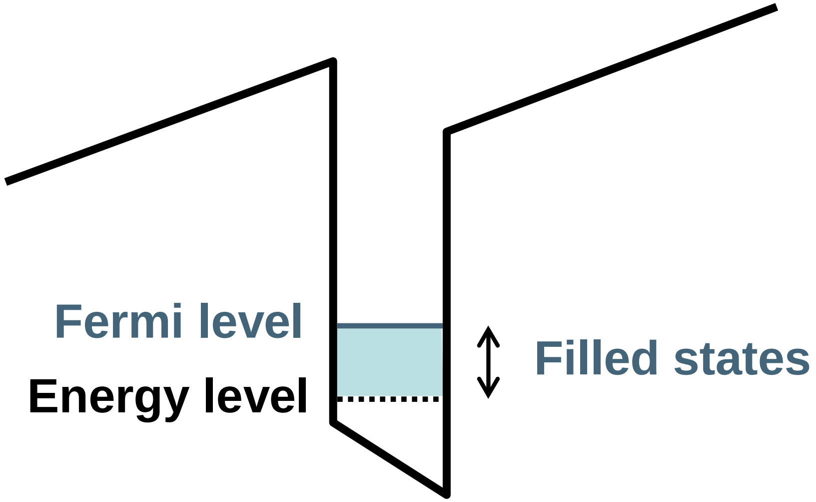


Quantum Effect 2:
Quantum Confinement in QWs

Classical description of the carrier concentration



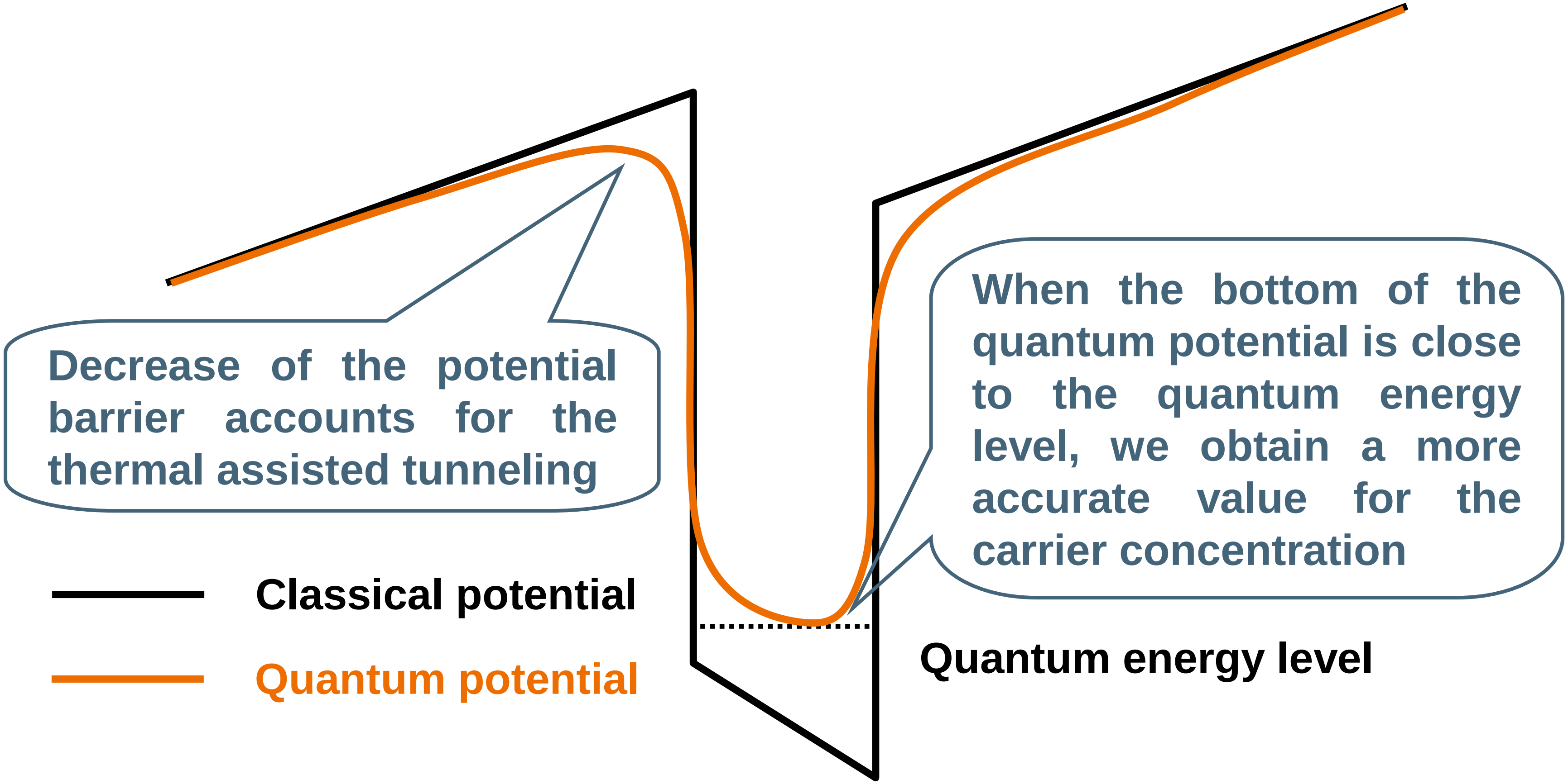
Quantum description of the carrier concentration



The same two-dimensional carrier concentration in a QW refers to a different Fermi level position for classical and quantum carrier description.

Solution For Both Quantum Effects:
Use of Quantum Potential

Quantum potential accounts approximately the quantum delocalization of the electrons/holes in a heterostructure with thin QWs and barriers, producing an effective band alignment used in the transport equations



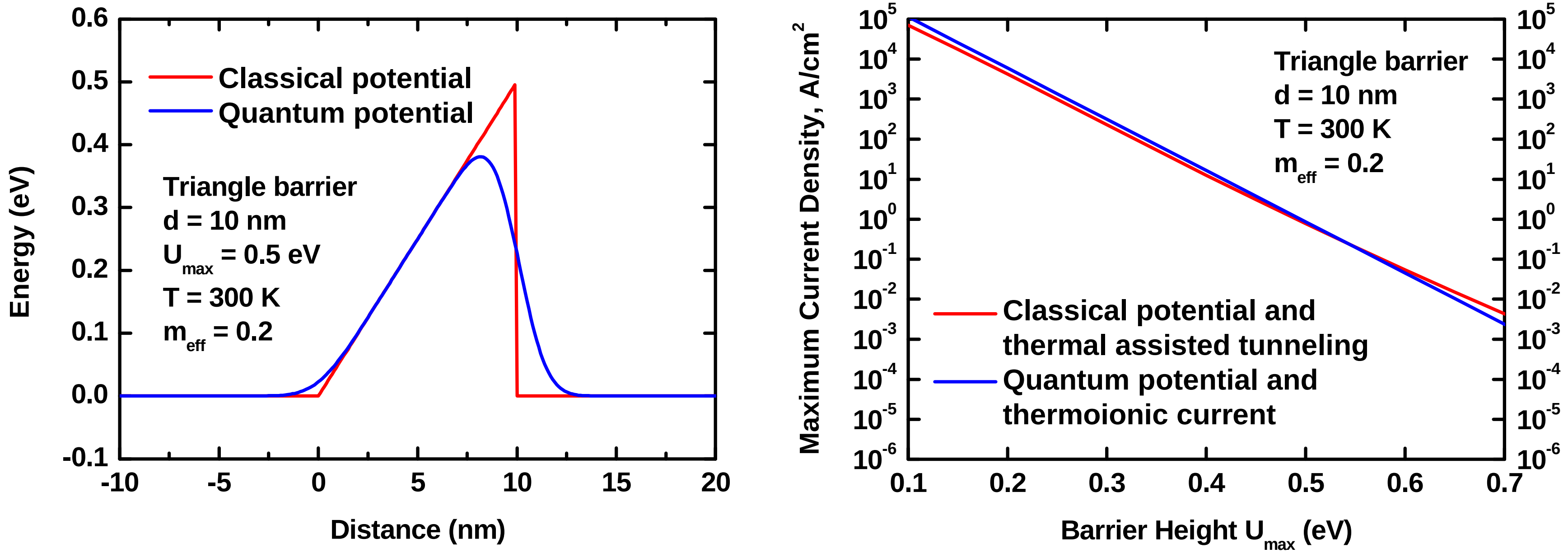
Decrease of the potential barrier accounts for the thermal assisted tunneling

When the bottom of the quantum potential is close to the quantum energy level, we obtain a more accurate value for the carrier concentration

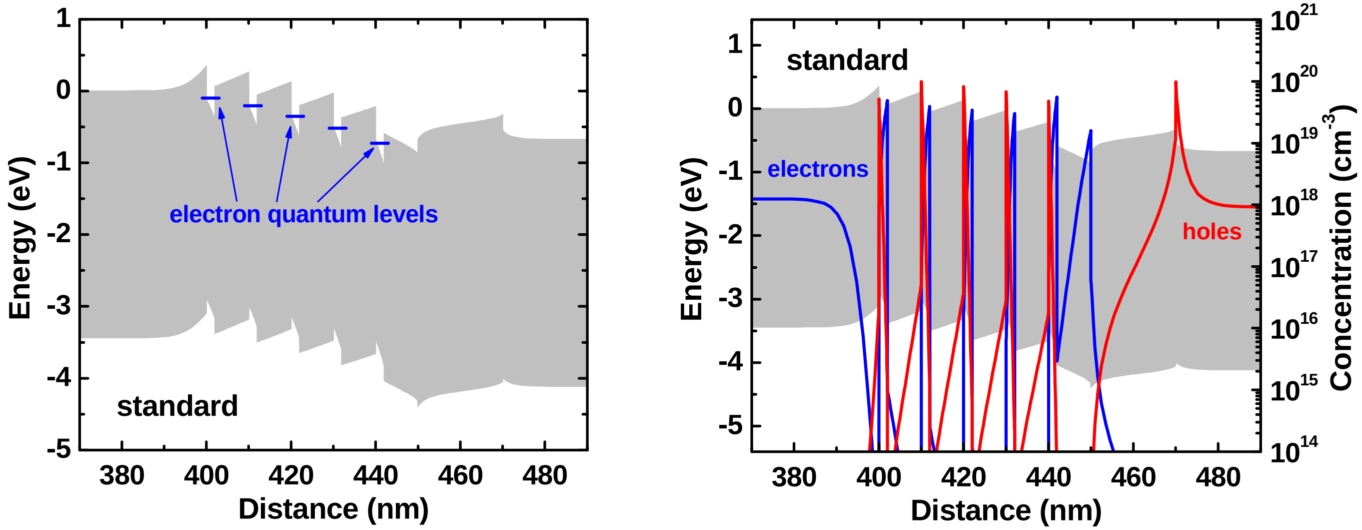
Model Verification

Analytical Estimation of Current Density

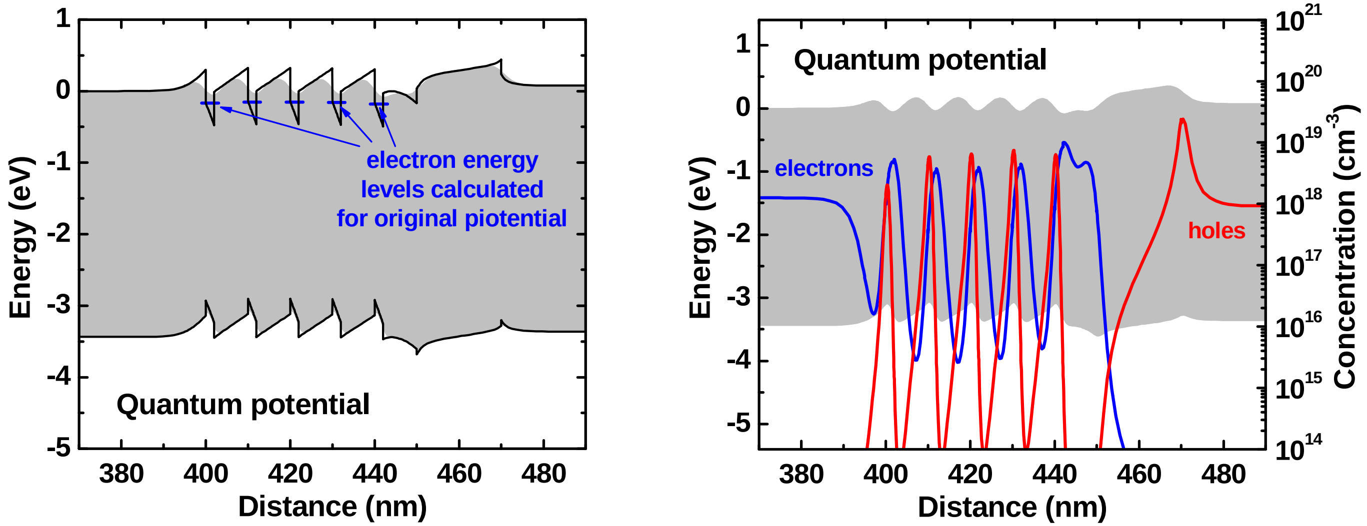
Thermo-ionic current density calculated with the quantum potential is in very good agreement with the tunnel current obtained from the original potential. This fact indicates that the quantum potential model provides reasonable estimation for the tunnel current density.



Model Prediction
Band Diagram and Carrier Distribution



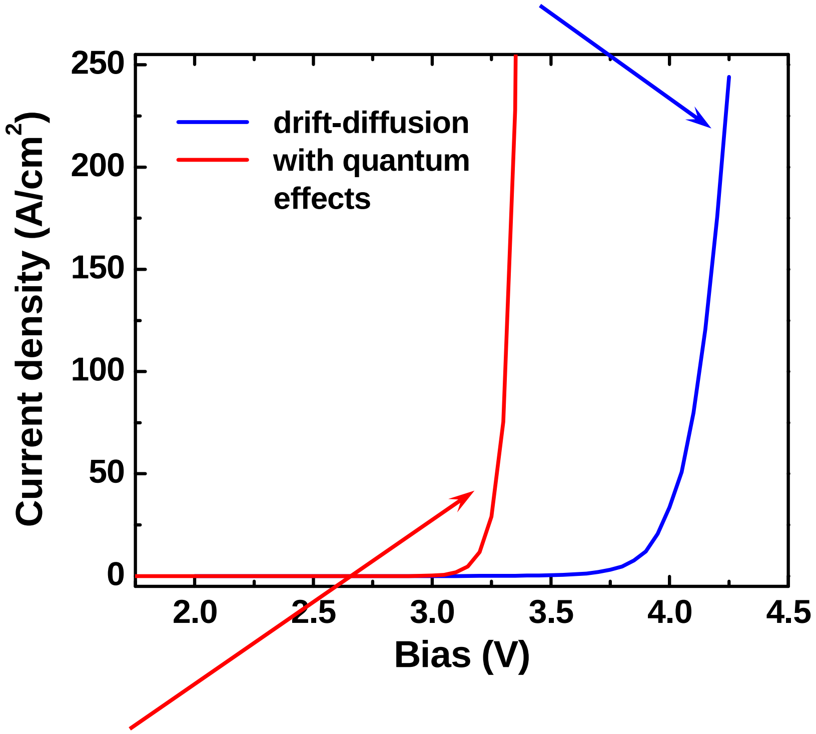
Drift-Diffusion



Quantum potential

Model Prediction
Improvement of I-V characteristics

Conventional drift-diffusion model overestimates the turn-on and operation voltage of MQW blue LEDs



Use of quantum potential improves predictability of the current-voltage characteristics for MQW blue LEDs