

# **Comparison of full-band Monte Carlo and Non-equilibrium Green's function simulations**

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# Motivation

- There is still a considerable separation between semi-classical and quantum models in terms of physical detail

strengths:

- advanced scattering models
- band structure readily included
- moderate computational cost

**Semi-classical  
transport**

particle

inclusion of:

- quantum corrections
- quantum sub-band details

strengths:

- quantum coherence
- tunneling and evanescent behavior at barriers

**Ballistic  
quantum  
transport**

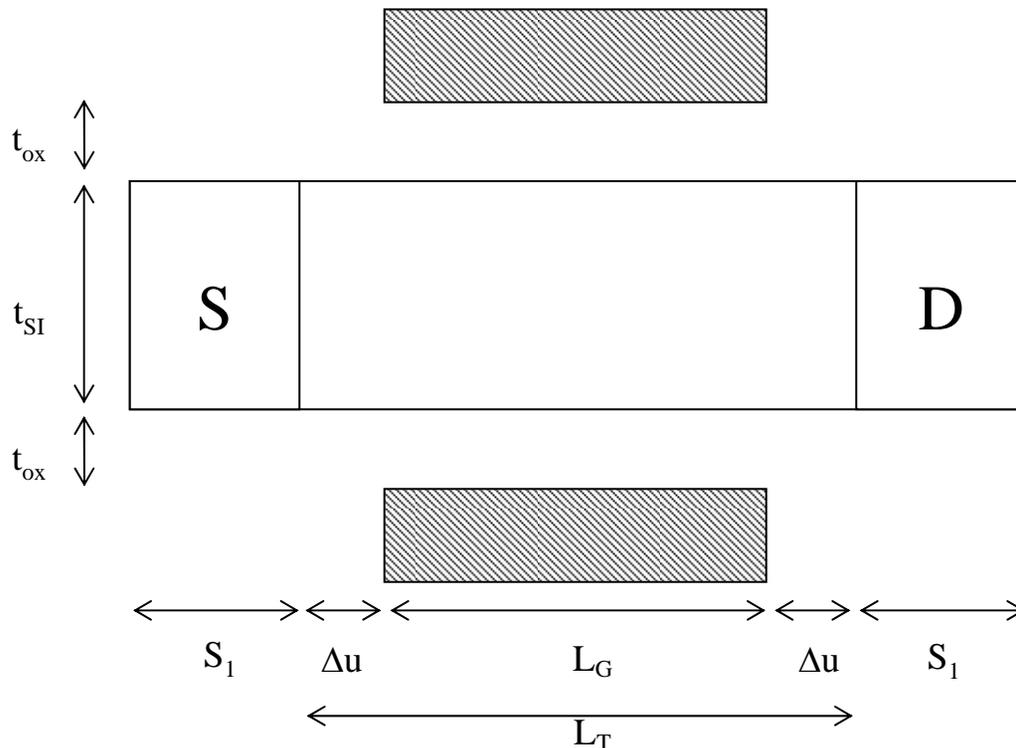
wave

inclusion of:

- scattering models
- band structure details

## Benchmark Model

- We have considered a 2-D device model for the double-gate MOSFET performing simulations with MOCA 2-D (UIUC) NanoMOS (Purdue).



### Device parameters

$$t_{ox} = 1.0 \text{ nm ( } k = 1.0 \text{ )}$$

$$t_{si} = 4.0 \text{ nm, } 3.0 \text{ nm, } 2.0 \text{ nm}$$

$$S_1 = 6.0 \text{ nm}$$

$$\Delta u = \text{underlap} = 4.0 \text{ nm}$$

$$L_G = 9.0 \text{ nm (-4.5nm to 4.5nm)}$$

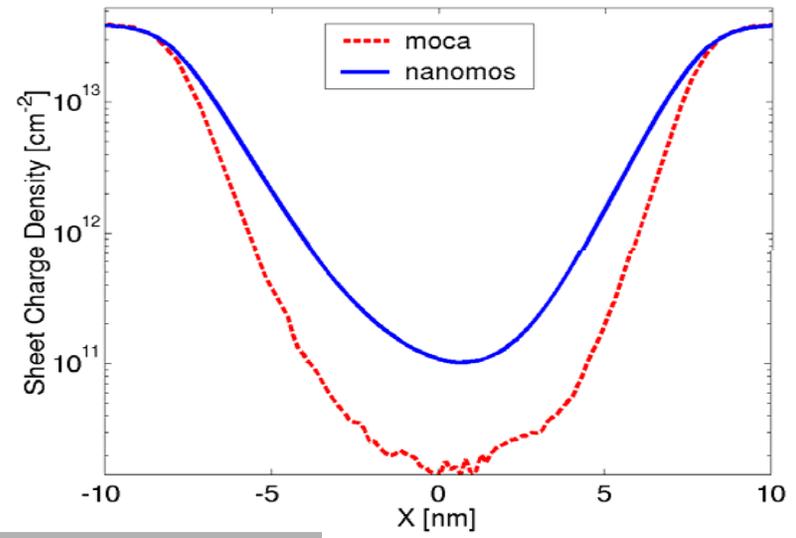
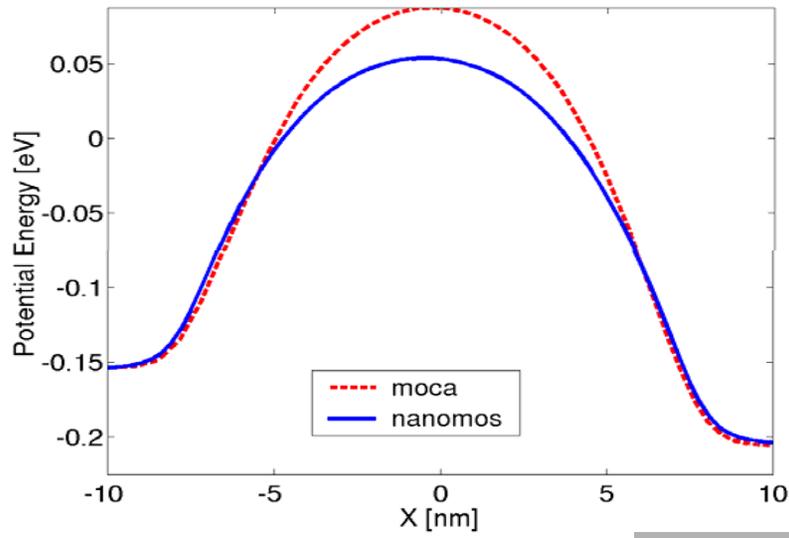
$$L_T = 17.0 \text{ nm (-8.5nm to 8.5nm)}$$

$$N_{S/D} = 10^{20} \text{ cm}^{-3}$$

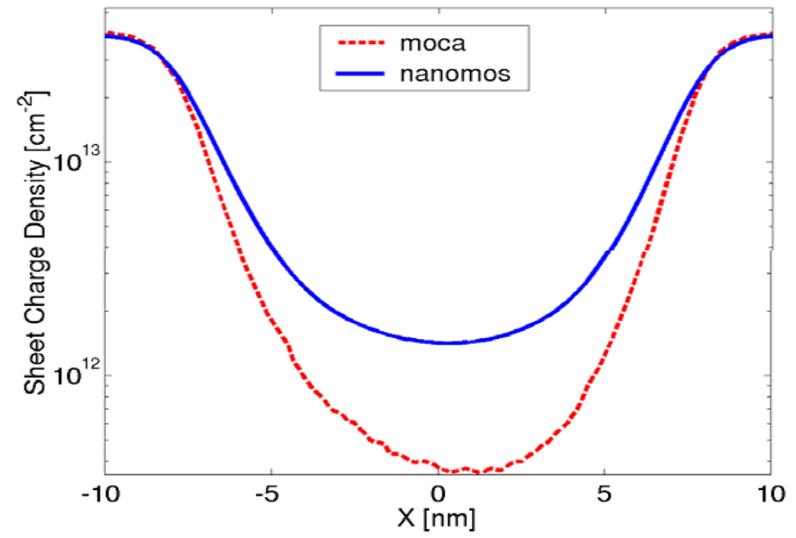
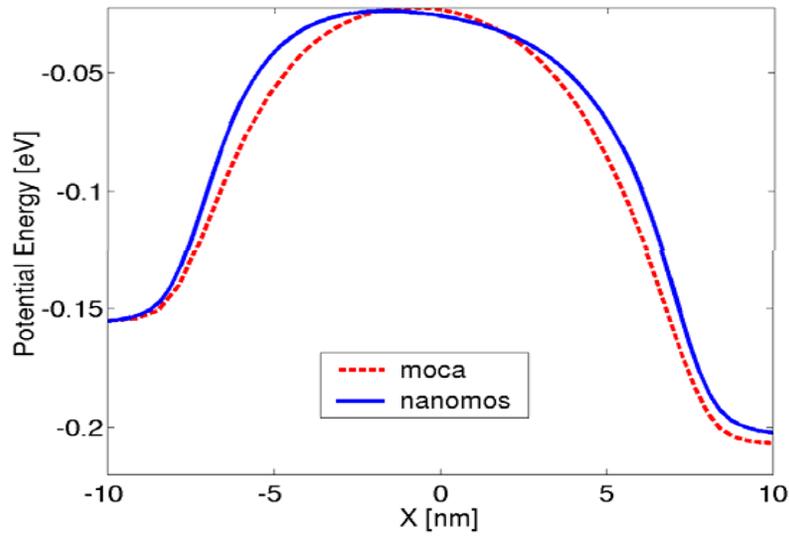
(gradient 1.0 nm/decade)

$$N_{body} = 10^{10} \text{ cm}^{-3}$$

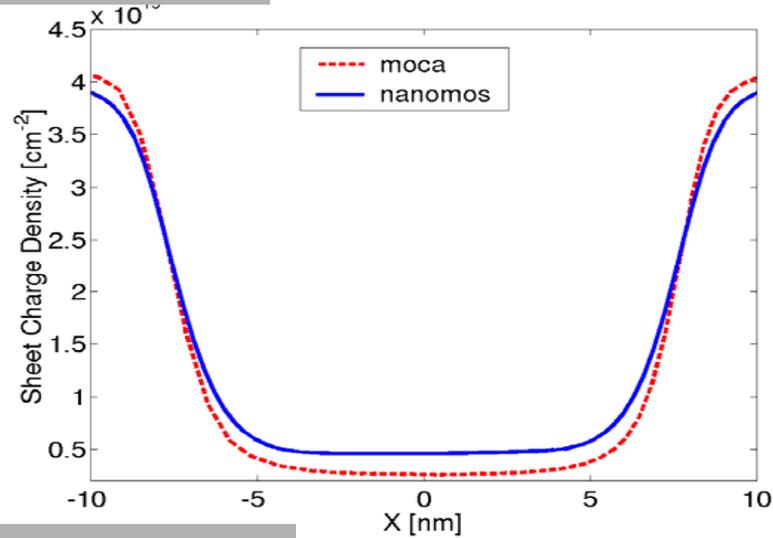
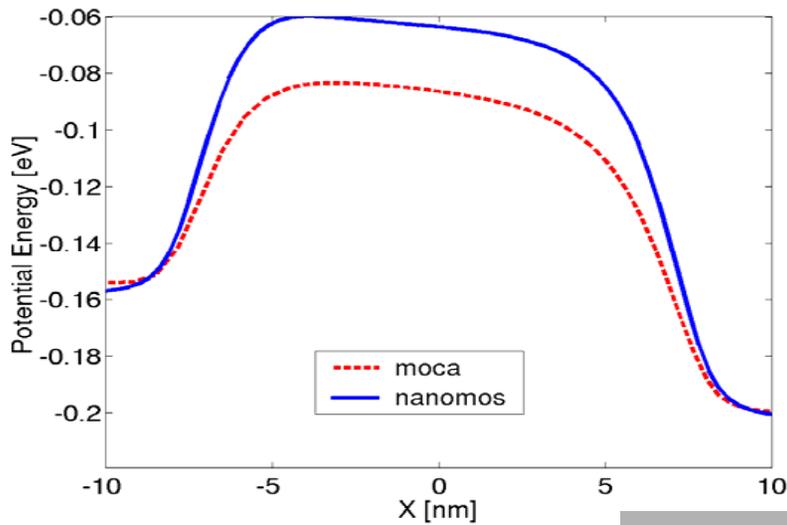
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.05\text{V}$ ,  $V_g = 0.05\text{V}$



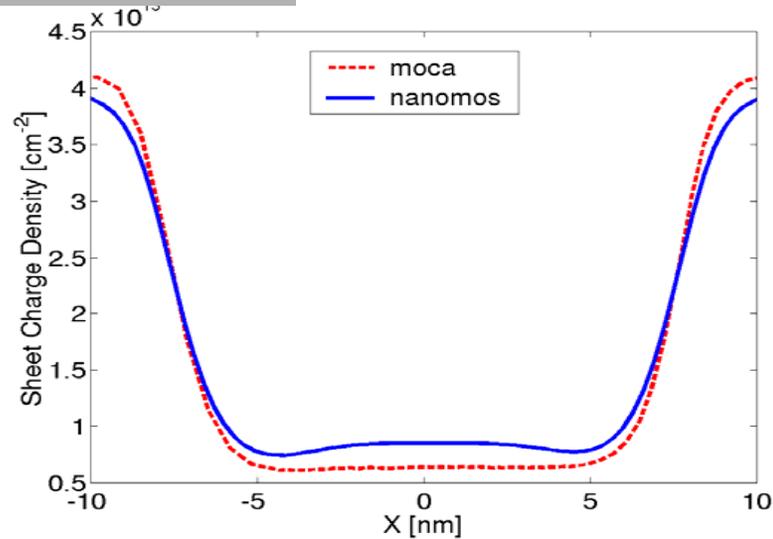
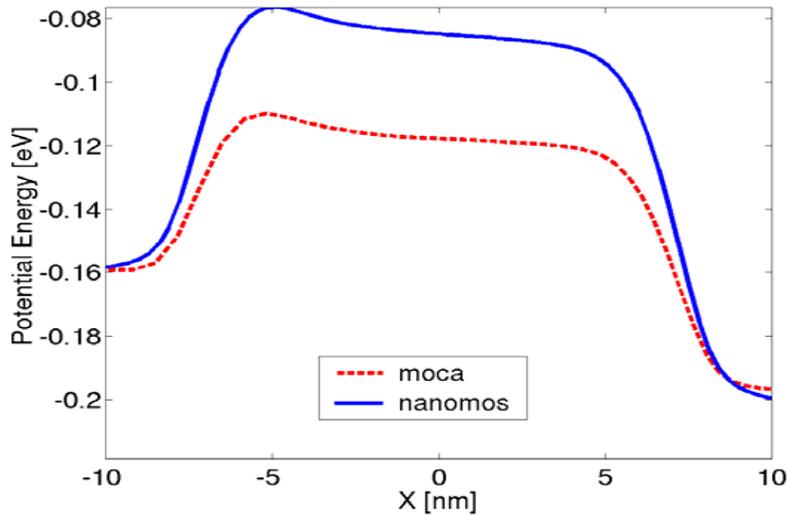
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.05\text{V}$ ,  $V_g = 0.20\text{V}$



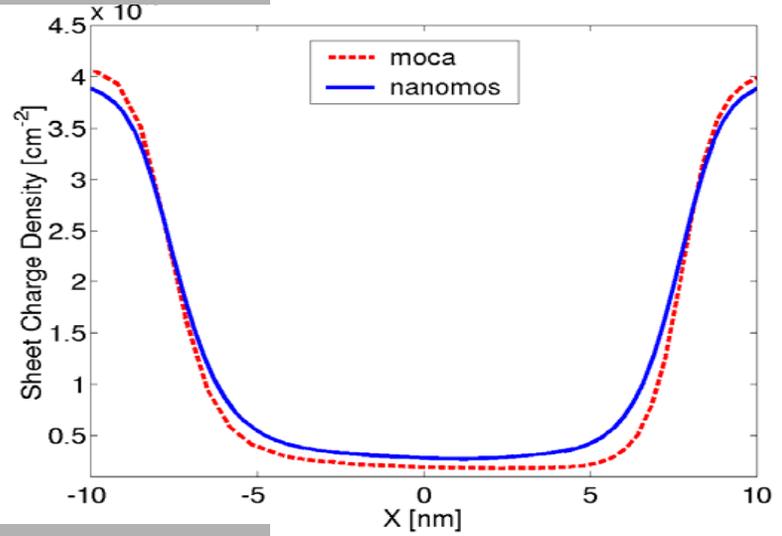
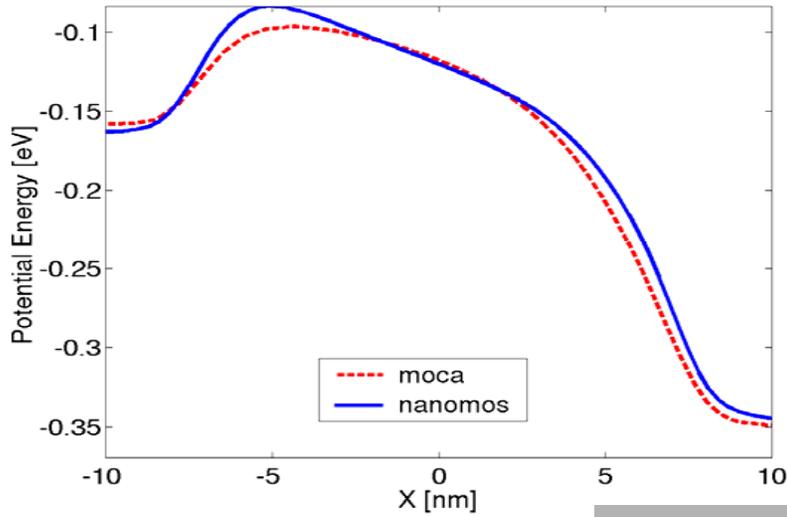
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.05\text{V}$ ,  $V_g = 0.35\text{V}$



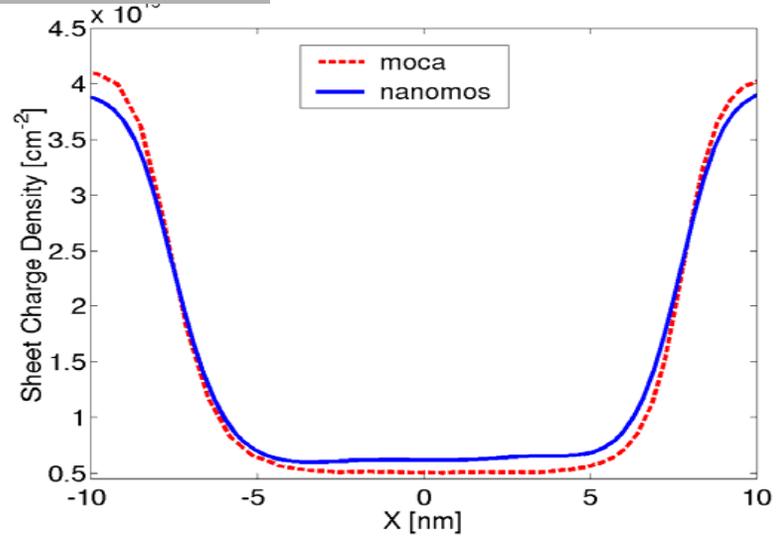
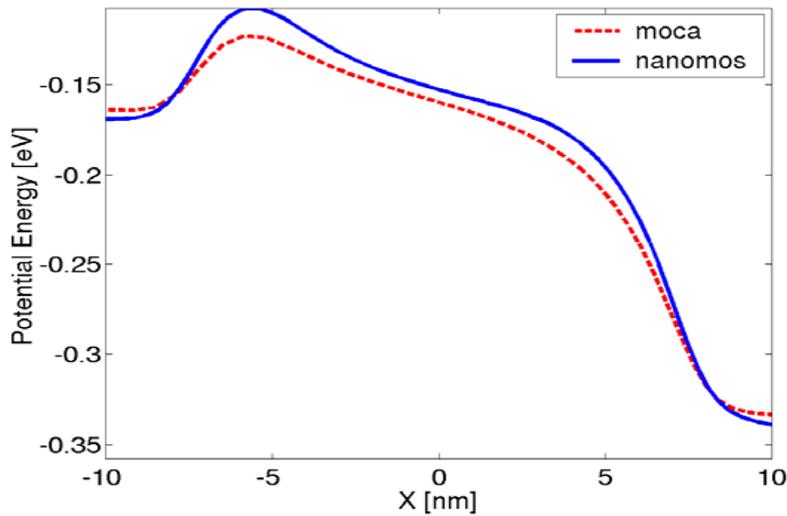
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.05\text{V}$ ,  $V_g = 0.50\text{V}$



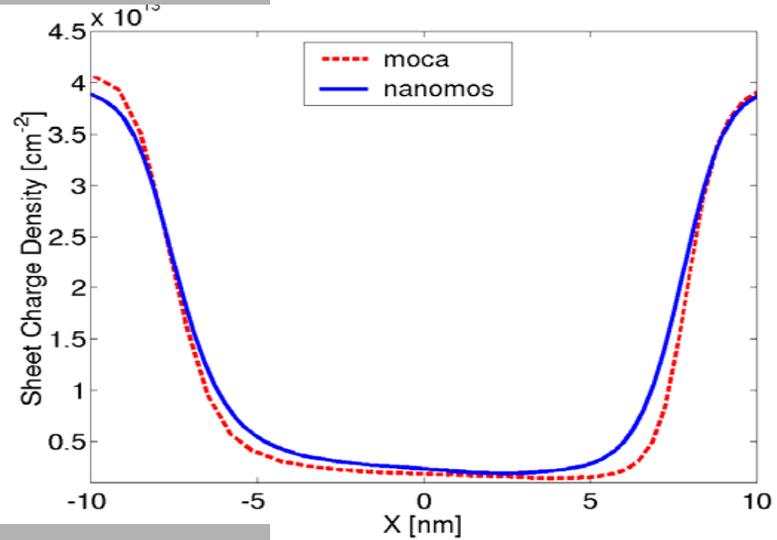
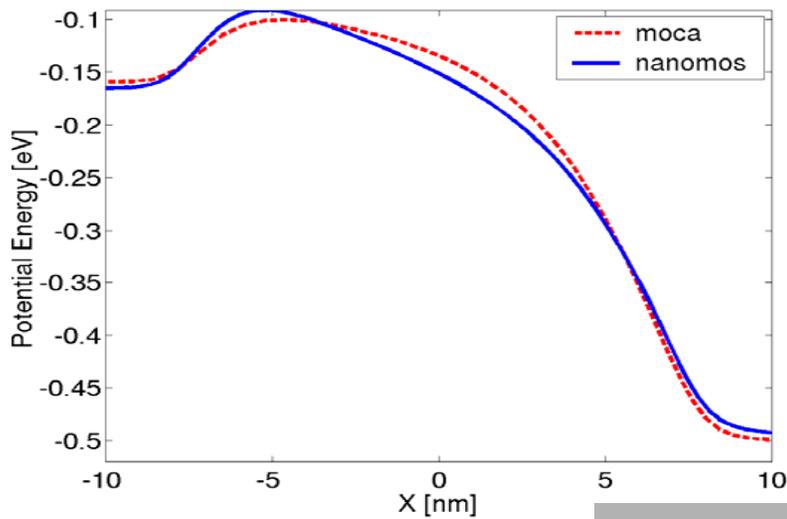
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.20\text{V}$ ,  $V_g = 0.35\text{V}$



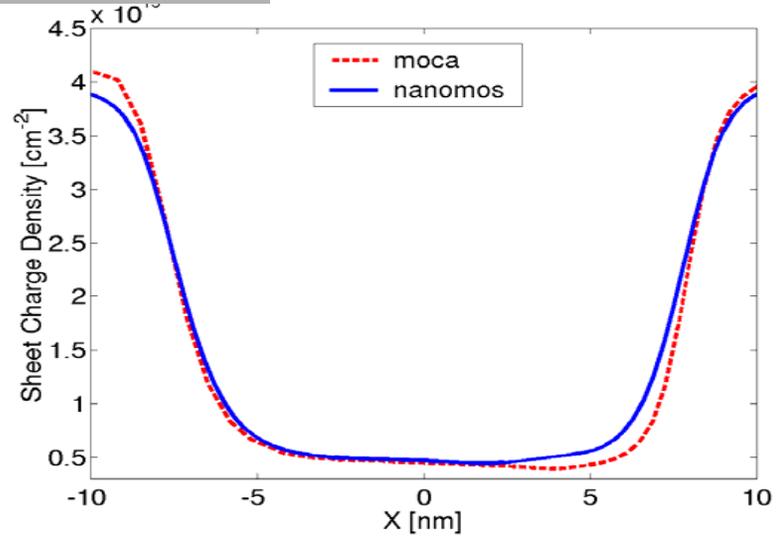
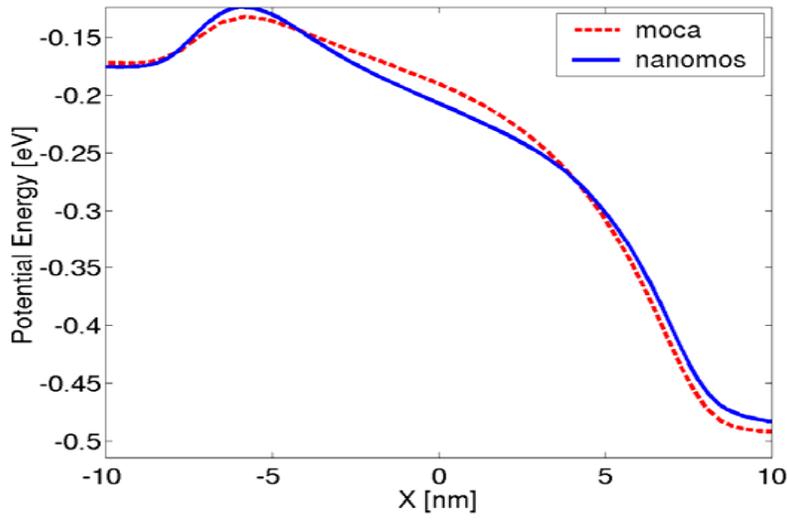
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.20\text{V}$ ,  $V_g = 0.50\text{V}$



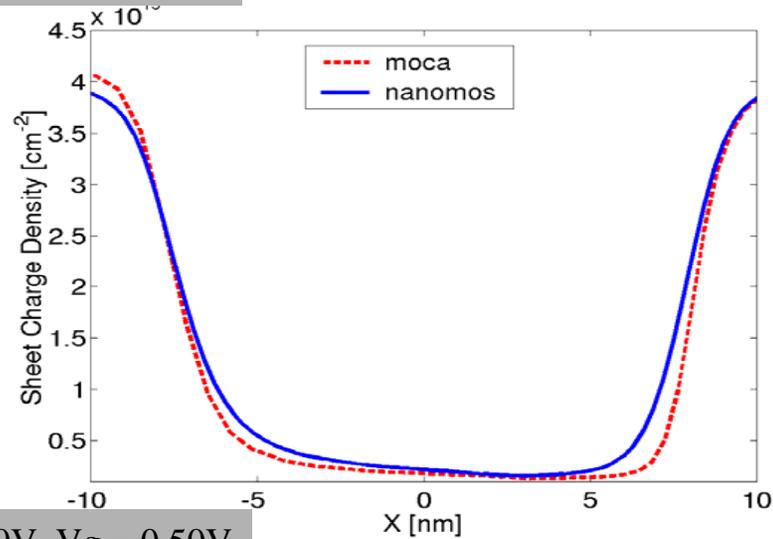
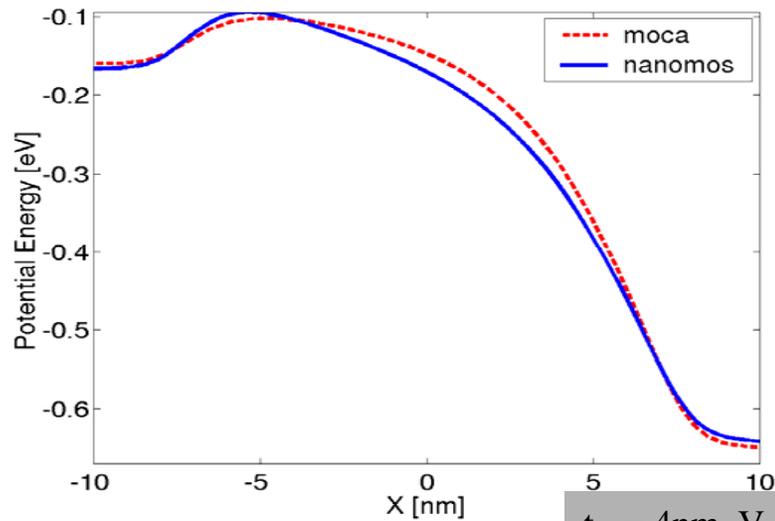
$t_{Si} = 4\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.35\text{V}$



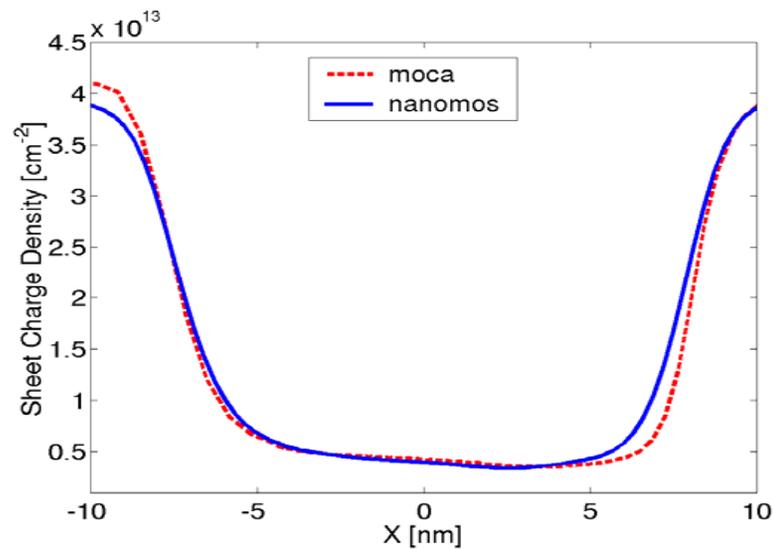
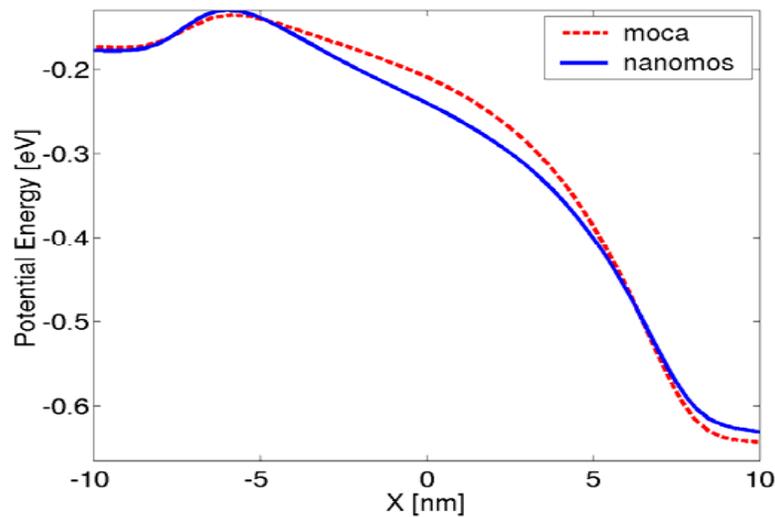
$t_{Si} = 4\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.50\text{V}$



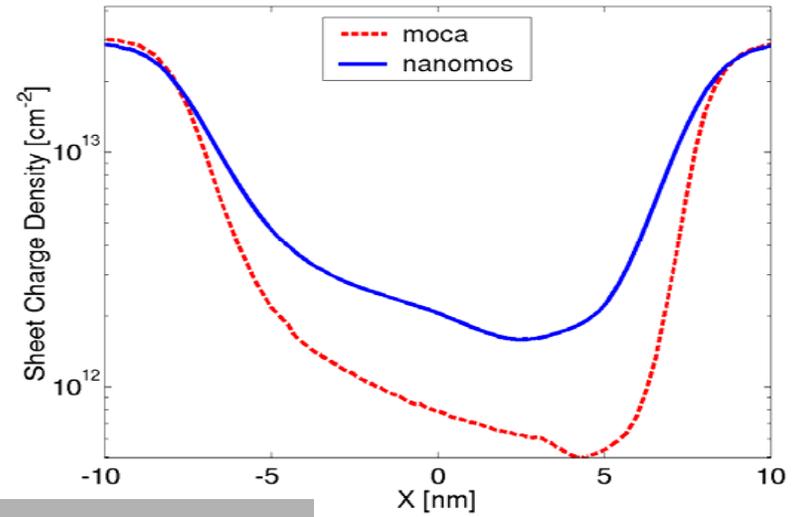
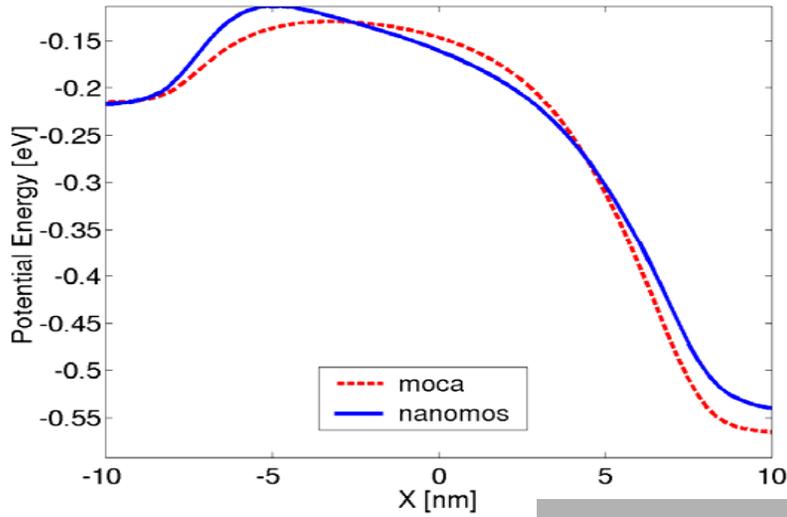
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.35\text{V}$



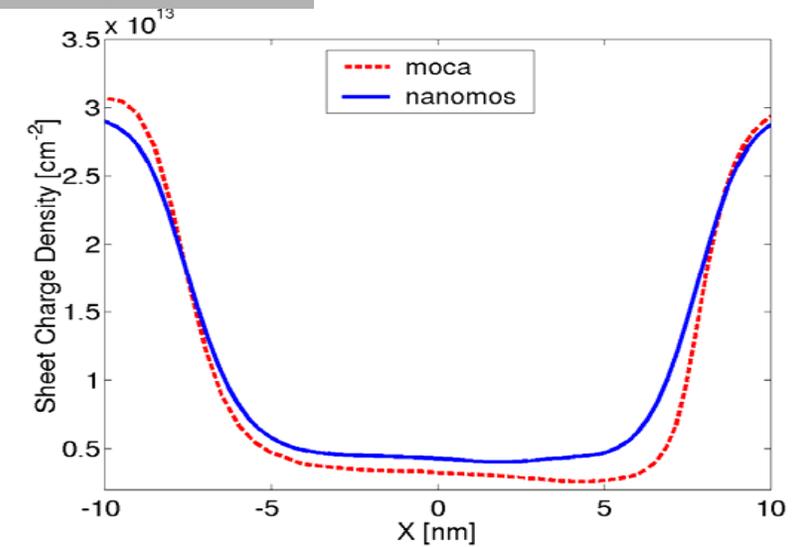
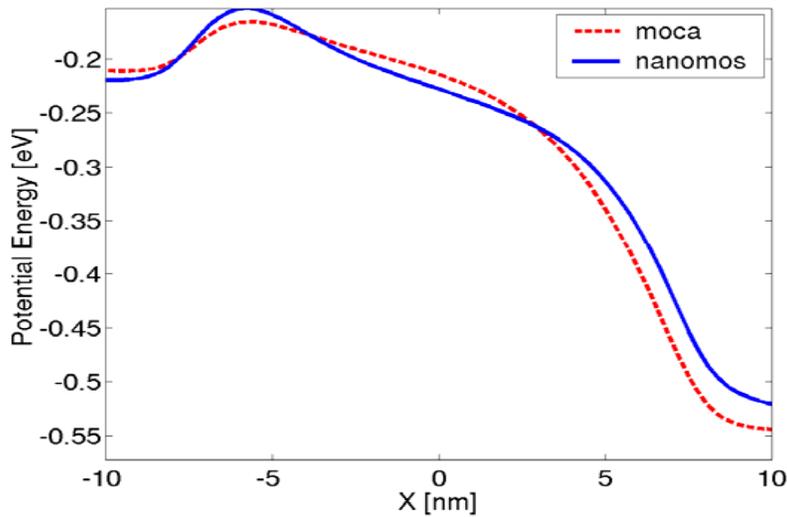
$t_{Si} = 4\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.50\text{V}$



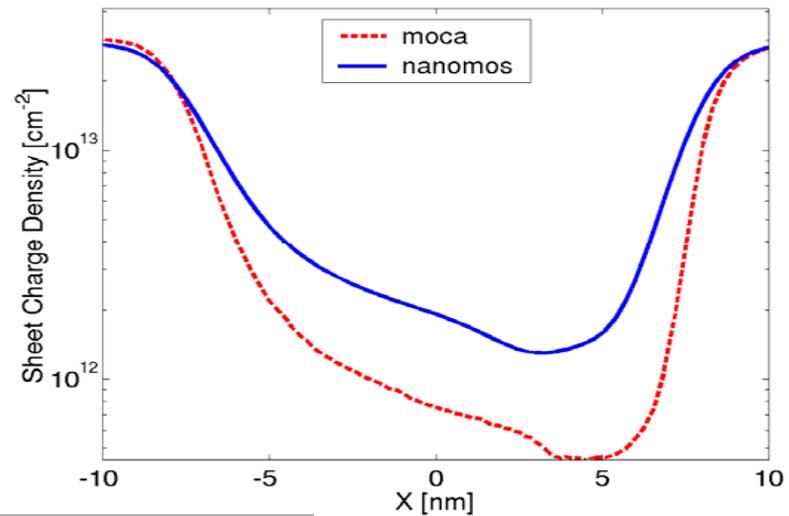
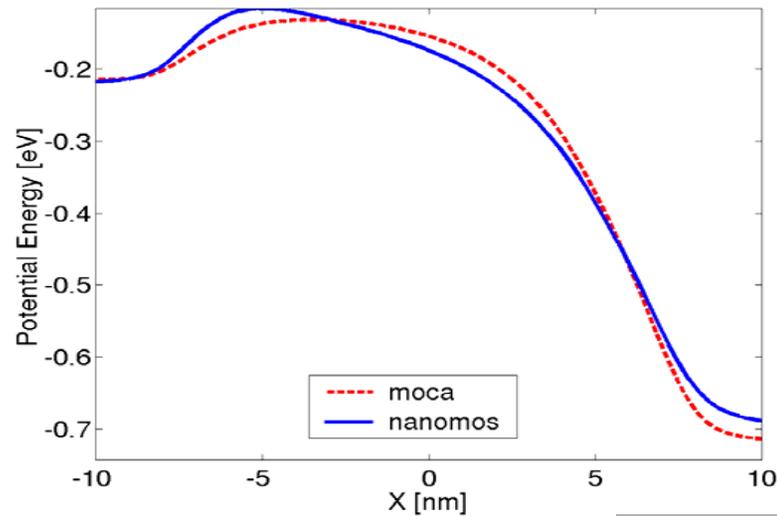
$t_{Si} = 3\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.35\text{V}$



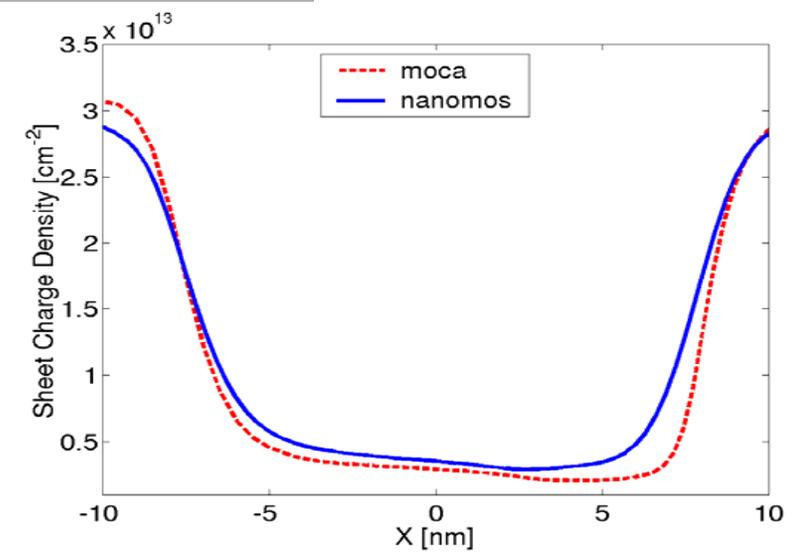
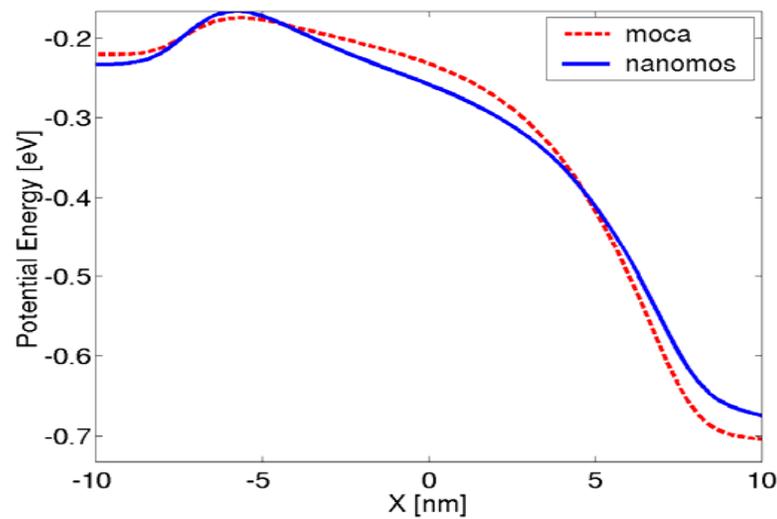
$t_{Si} = 3\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.50\text{V}$



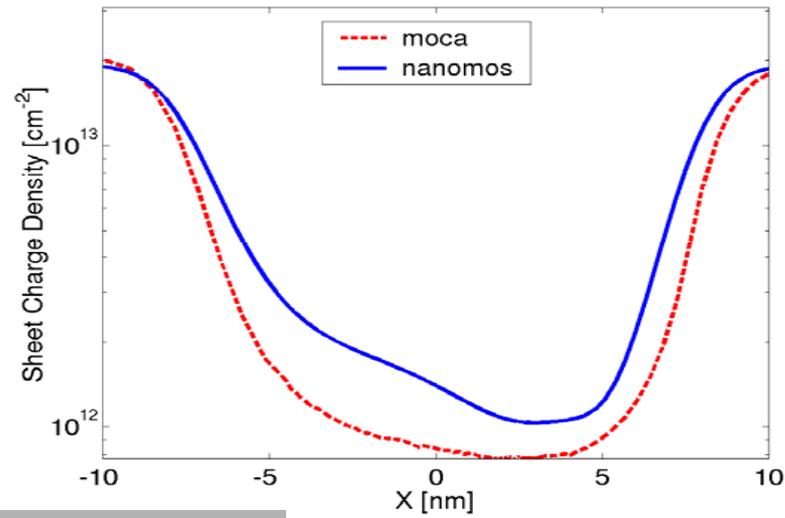
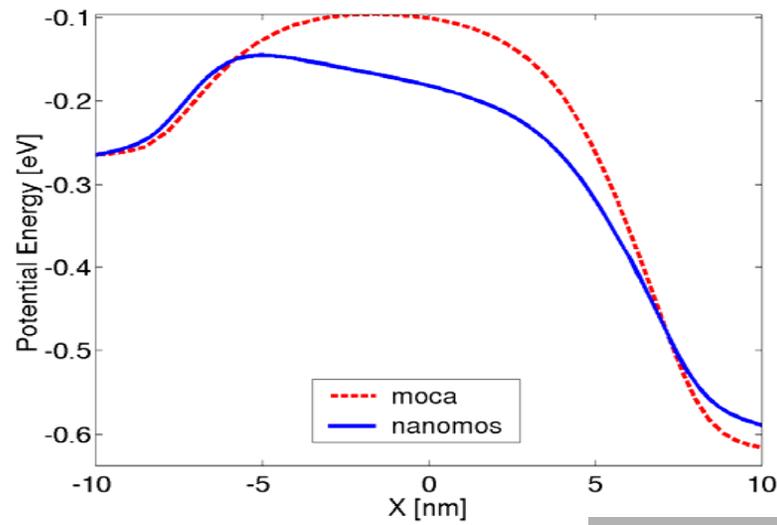
$t_{Si} = 3\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.35\text{V}$



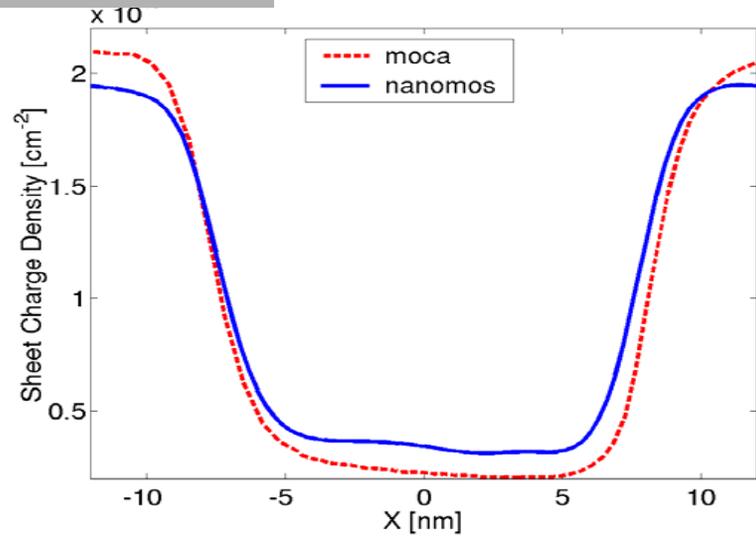
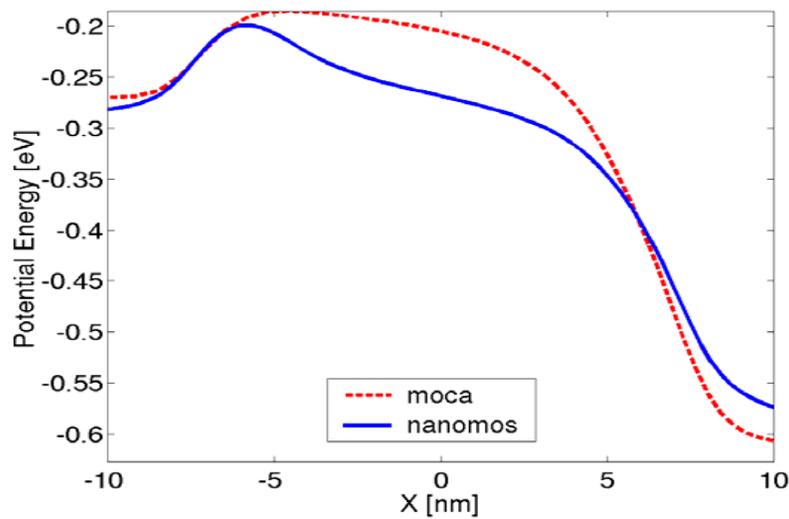
$t_{Si} = 3\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.50\text{V}$



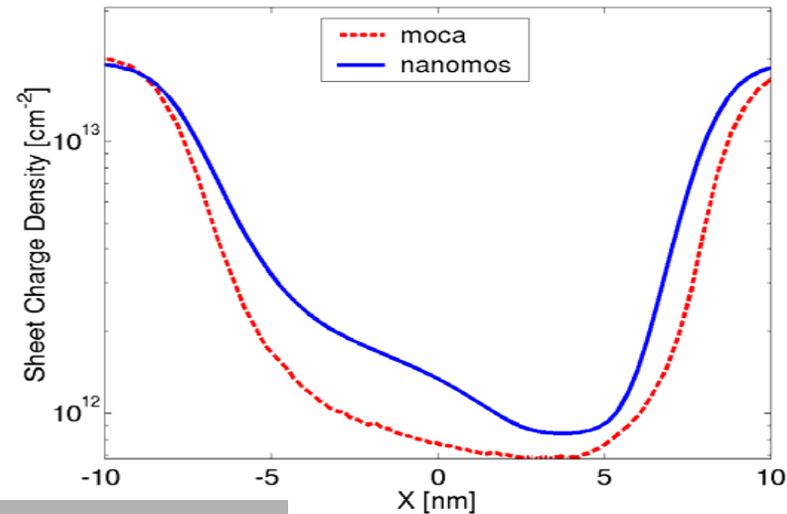
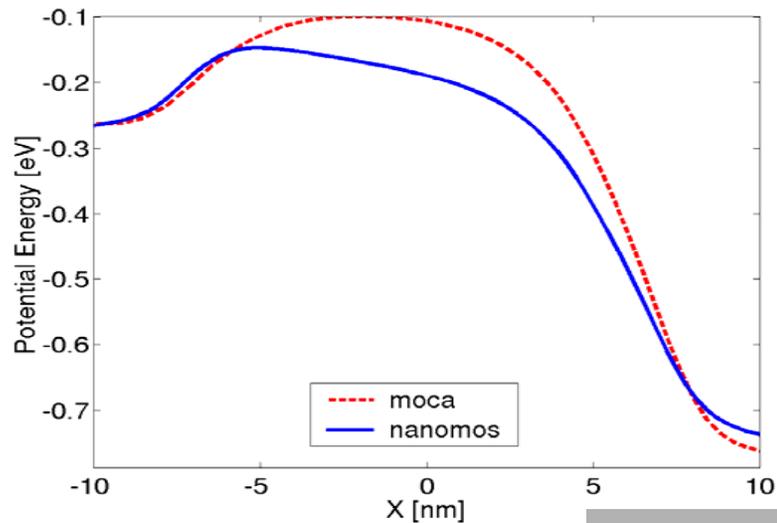
$t_{Si} = 2\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.35\text{V}$



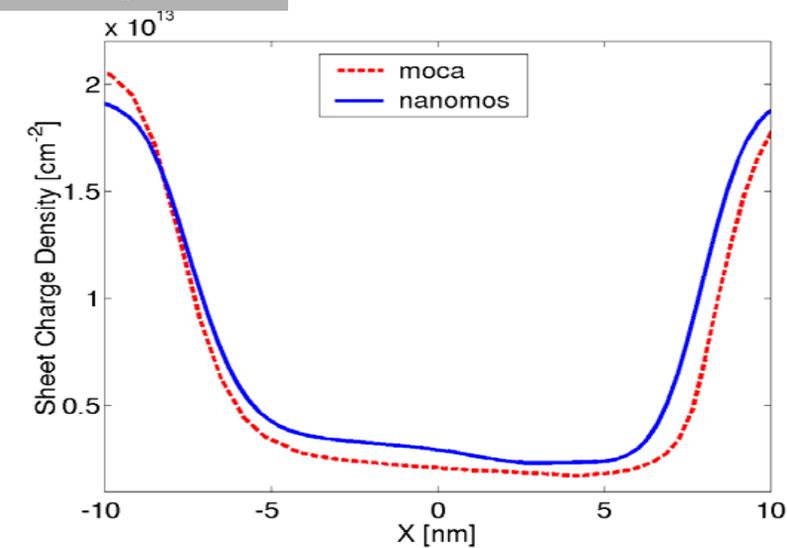
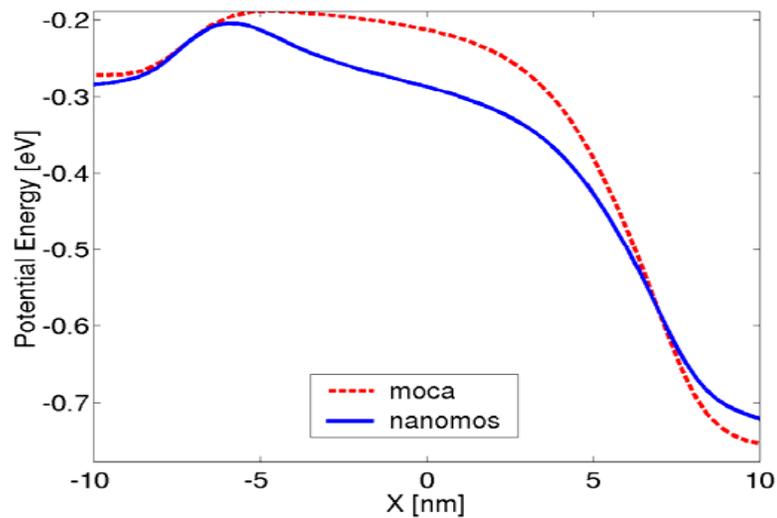
$t_{Si} = 2\text{nm}, V_{ds} = 0.35\text{V}, V_g = 0.50\text{V}$

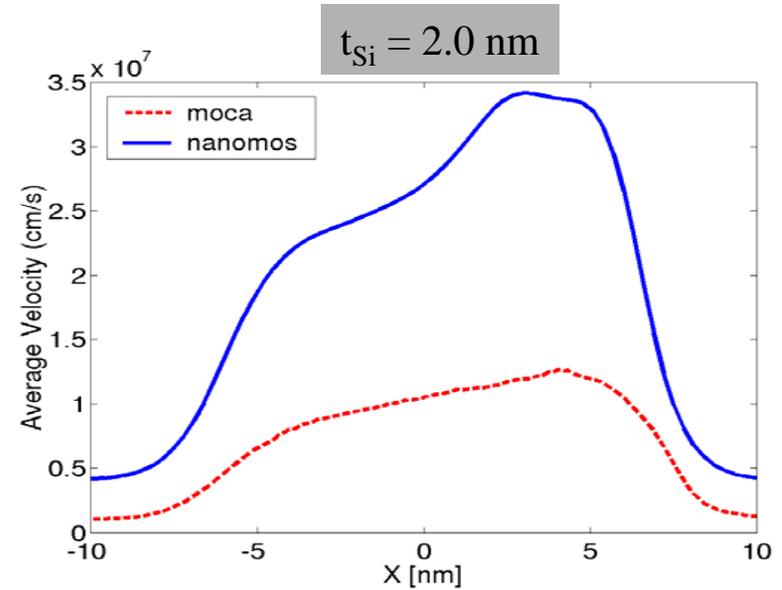
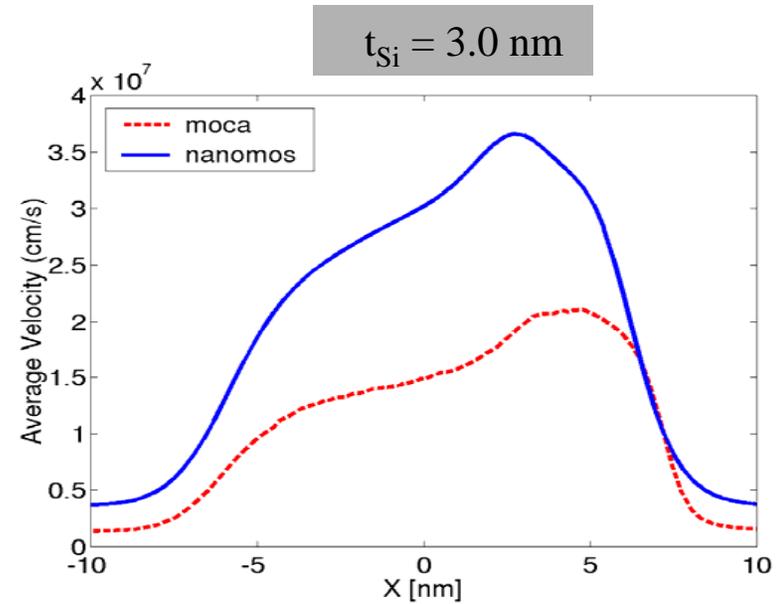
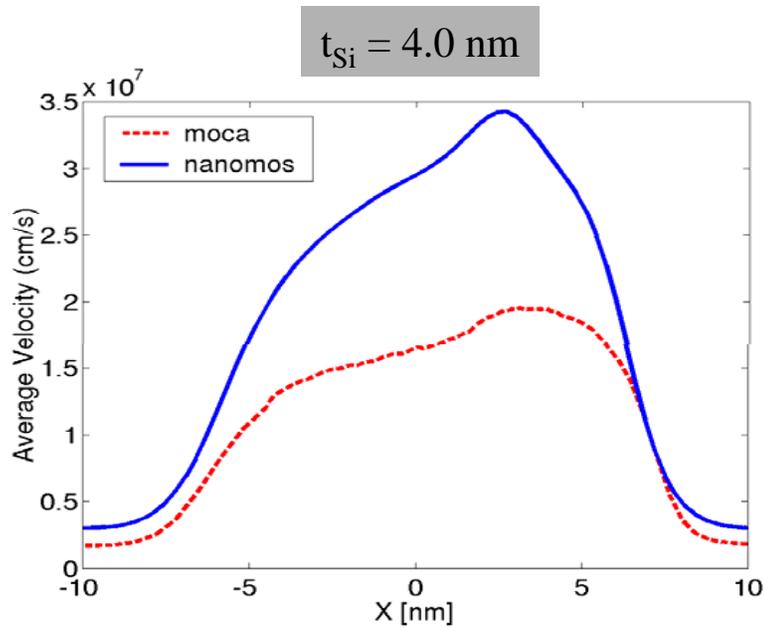


$t_{Si} = 2\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.35\text{V}$



$t_{Si} = 2\text{nm}$ ,  $V_{ds} = 0.50\text{V}$ ,  $V_g = 0.50\text{V}$

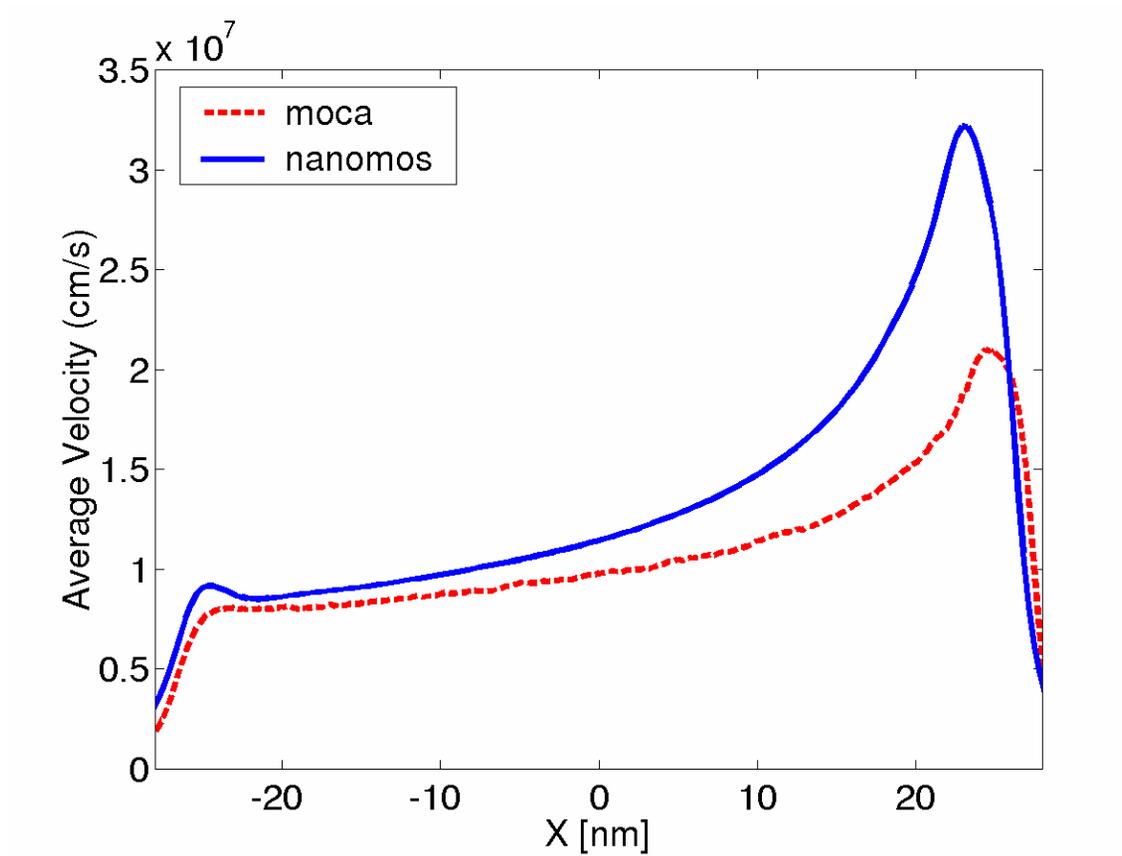




**Velocity Profiles**  
 $V_{ds} = 0.50V, V_g = 0.50V$

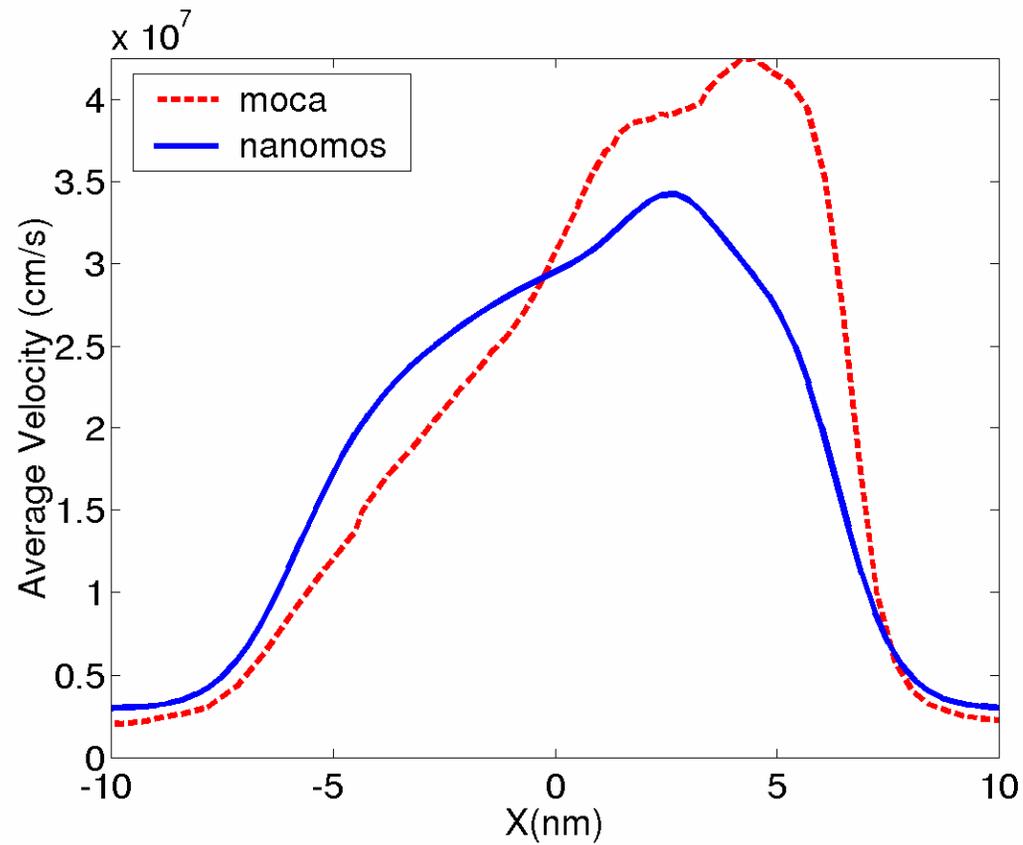
## Long Channel benchmark

$t_{\text{Si}} = 3.0 \text{ nm}$   $L_G = 50 \text{ nm}$ ,  $V_{\text{ds}} = 0.50\text{V}$ ,  $V_g = 0.50\text{V}$



## Velocity comparison for a ballistic device

$t_{Si} = 4.0 \text{ nm}$   $L_G = 9 \text{ nm}$ ,  $V_{ds} = 0.50 \text{ V}$ ,  $V_g = 0.50 \text{ V}$



# Conclusions

- The present benchmark comparison indicates that Monte Carlo and NEGF simulations give potential and density profiles that agree well in a range of conditions and silicon slab thicknesses.
- Discrepancies are noticed at low bias, explained by the granular nature of Monte Carlo as opposed to the continuum nature of NEGF.
- For thinner silicon slab thickness, size quantization is emphasized, and we are looking for the limits of validity of the quantum correction potential approach in Monte Carlo.
- At high fields, NEGF tend to give a much more prominent velocity overshoot. This is understood by considering that the present model of nanoMOS has parabolic bands, where velocity is not constrained as in a realistic band.