# Exercises:
# 1) Formation of Bandstructure in Finite Superlattices
# 2) RTDs

Gerhard Klimeck

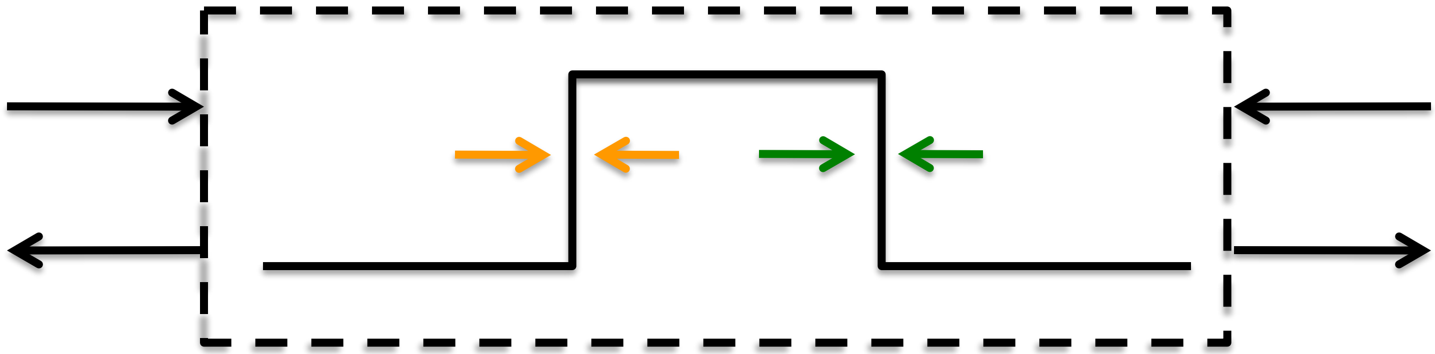
NCN

- Analytical solutions of Toy Problems
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers

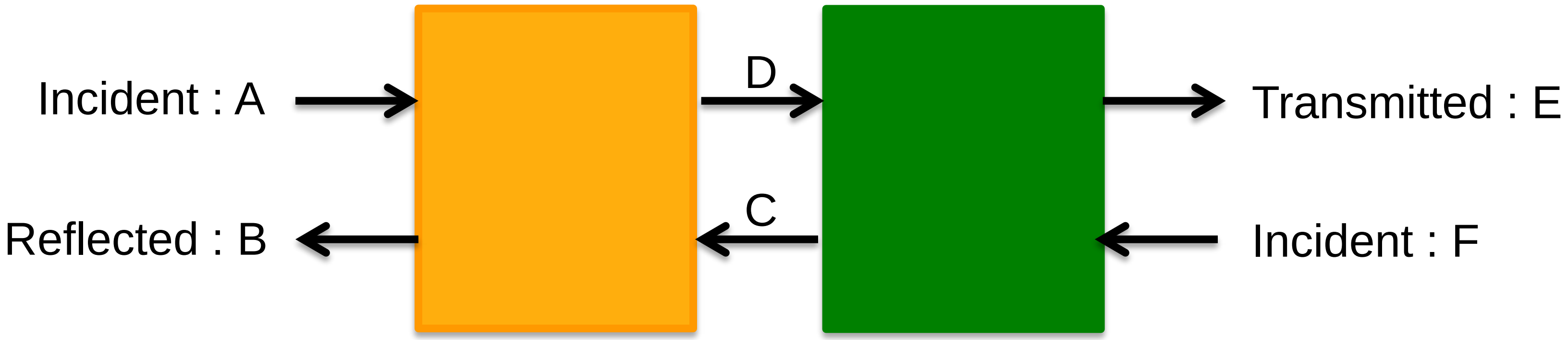
**Reference:**

- piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt

Define our system : Single barrier

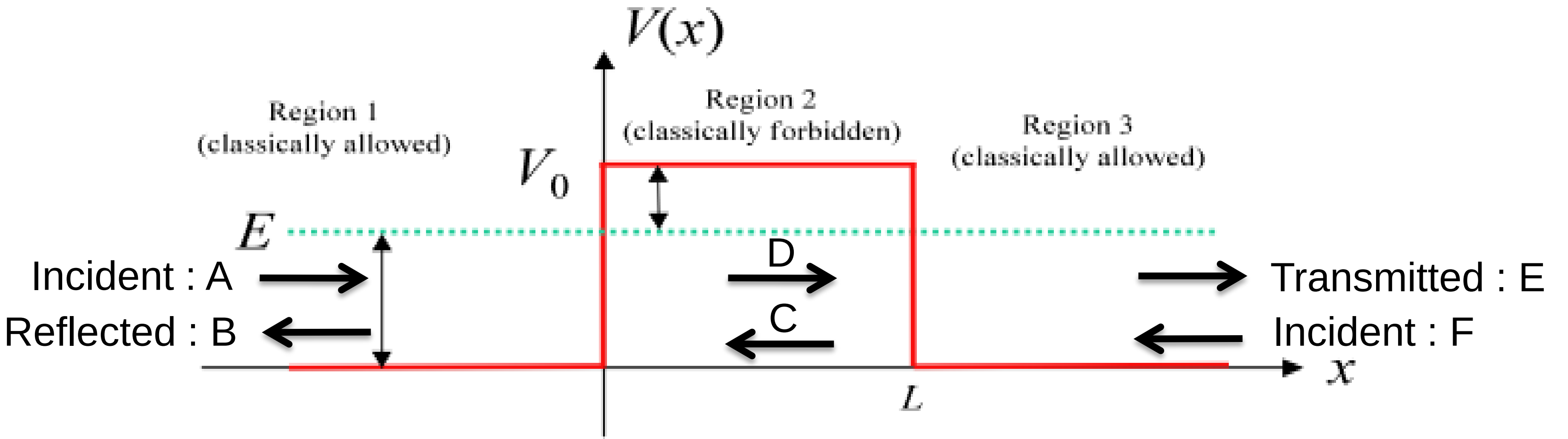


One matrix each for each interface: 2 S-matrices




No particles lost! Typically A=1 and F=0.

# Tunneling through a single barrier




Wave-function each region,

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2(x) = Ce^{-\gamma x} + De^{\gamma x}$$

$$\psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \gamma = \sqrt{\frac{2m\left(V_0 - E\right)}{\hbar^2}}$$

# Single barrier case

Applying boundary conditions at each interface (x=0 and x=L) gives,

$$\psi_1(0) = \psi_2(0) \quad \rightarrow \quad A + B = C + D$$

$$\psi_1'(0) = \psi_2'(0) \quad \rightarrow ik(A - B) = -\gamma(C - D)$$

$$\psi_2(L) = \psi_3(L) \quad \rightarrow \quad Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL}$$

$$\psi_2'(L) = \psi_3'(L) \quad \rightarrow \quad -\gamma\left(Ce^{-\gamma L} - De^{\gamma L}\right) = ik\left(Ee^{ikL} - Fe^{-ikL}\right)$$

Which in matrix can be written as,

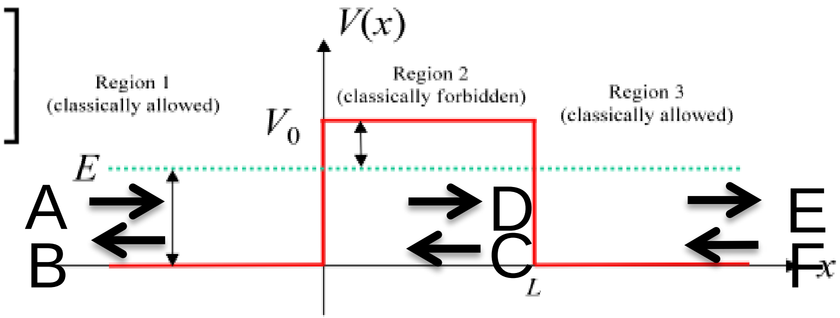
$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) \\ \frac{1}{2}\left(1 - i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1 + i\frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{(ik+\gamma)L} & \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{-(ik-\gamma)L} \\ \frac{1}{2}\left(1 + i\frac{k}{\gamma}\right)e^{(ik-\gamma)L} & \frac{1}{2}\left(1 - i\frac{k}{\gamma}\right)e^{-(ik+\gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}$$

# Generalization to Transfer Matrix Method

- The complete transfer matrix

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix}$$




- In general for any intermediate set of layers, the TMM is expressed as:

$$\begin{pmatrix} A_{n-1}^{+} \\ A_{n-1}^{-} \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_n^{+} \\ A_n^{-} \end{pmatrix}$$

- For multiple layers the overall transfer matrix will be

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \prod_{j=2..N} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Looks conceptually very simple and analytically pleasing
- Use it for your homework assignment for a double barrier structure!

# Single barrier case

Transmission can be found using the relations between unknown constants,

$$\begin{bmatrix} A \\ B \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix} = M_1 M_2 \begin{bmatrix} E \\ F \end{bmatrix} = M \begin{bmatrix} E \\ F \end{bmatrix} \qquad T(E) = \left| \frac{E}{A} \right|^2 = \frac{1}{|m_{11}|^2}$$

Case: E<$V_o$

$$T(E) = \left[ 1 + \left( \frac{\gamma^2 + k^2}{2k\gamma} \right)^2 sh^2(\gamma L) \right]^{-1}$$

Case($\gamma L$ large): Strong barrier

$$T(E) \approx \left( \frac{4k\gamma}{k^2 + \gamma^2} \right)^2 \exp(-2\gamma L)$$

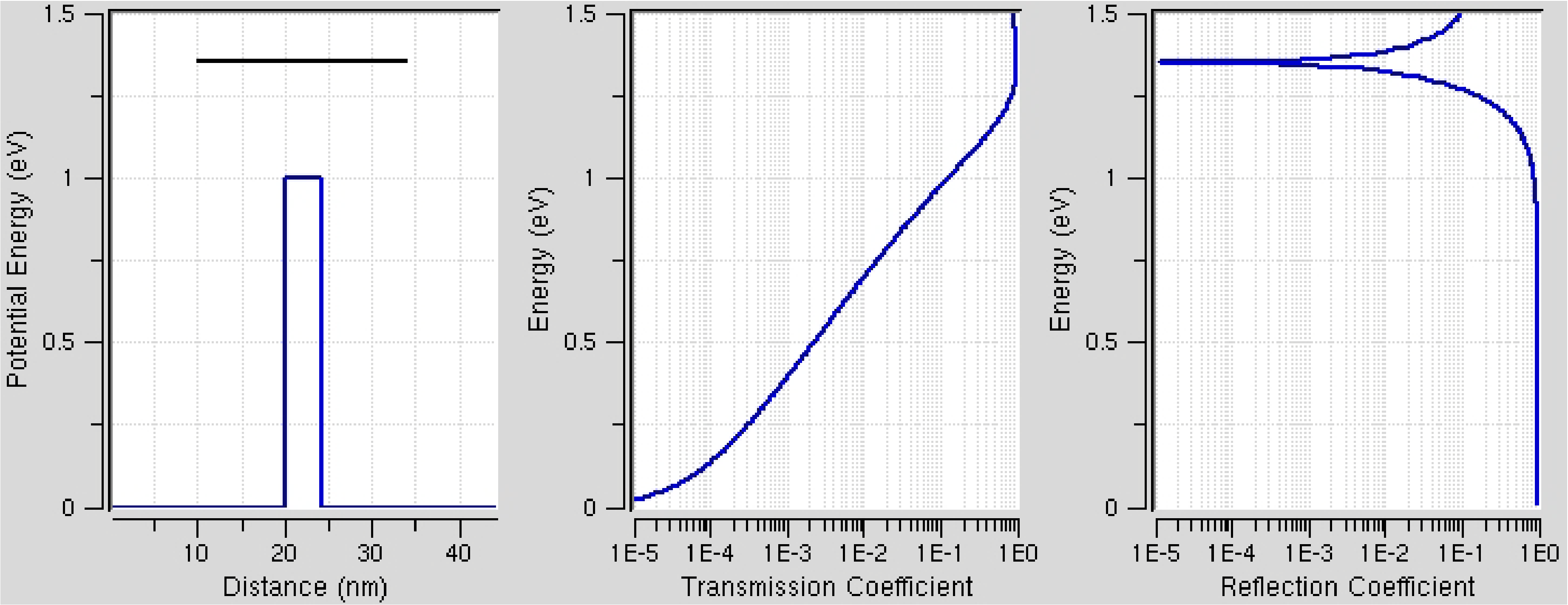
Case($\gamma L$<<1): Weak barrier

$$T(E) \approx \frac{1}{1 + (kL/2)^2}$$

Case: E>$V_o$

$$T(E) = \left[ 1 + \left( \frac{k^2 - k_2^2}{2kk_2} \right)^2 \sin^2(k_2 L) \right]^{-1}$$

# Single barrier : Concepts



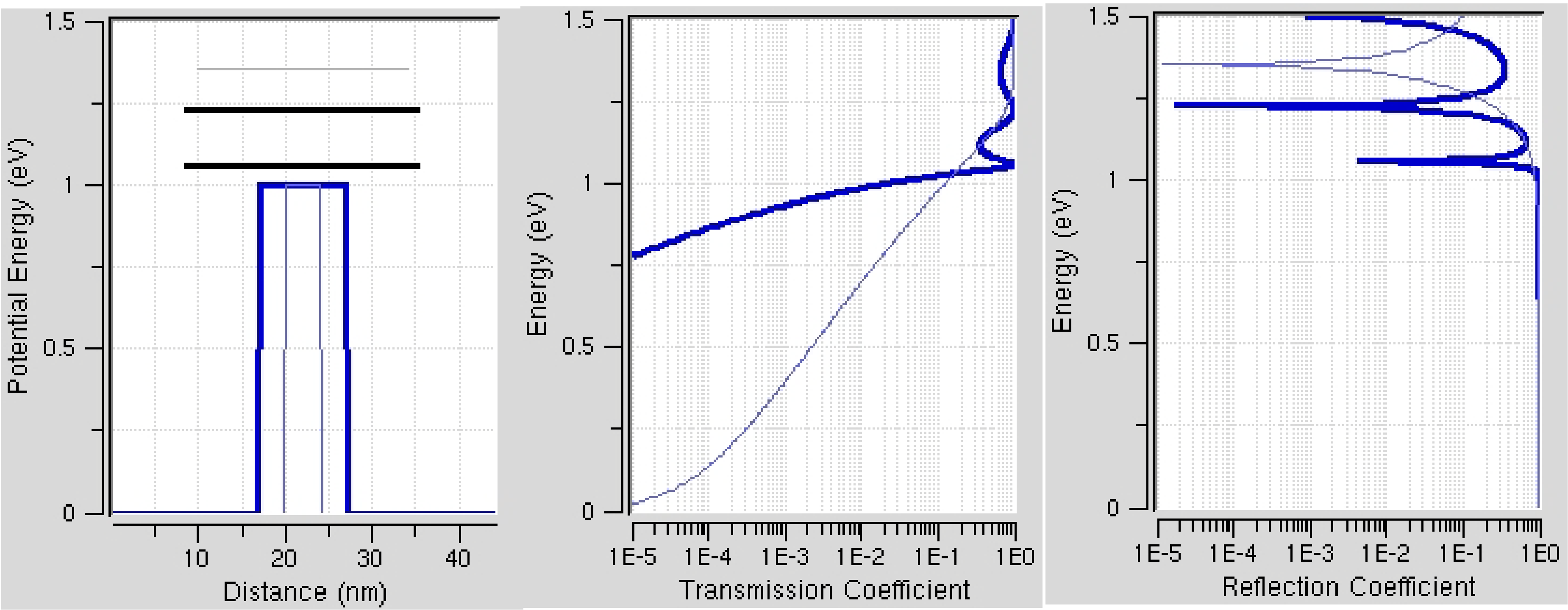

- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier. Transmission goes to one.

Case: $E>V_o$

$$T(E) = \left[ 1 + \left( \frac{k^2 - k_2^2}{2kk_2} \right)^2 \sin^2(k_2 L) \right]^{-1}$$

- Computed with – http://nanohub.org/tools/pcpbt

# Effect of barrier thickness below the barrier




- Increased barrier width reduces tunneling probability
- Thicker barrier increase the reflection probability below the barrier height.
- Quasi-bound states occur for the thicker barrier too.
- Computed with – http://nanohub.org/tools/pcpbt

Case: $E>V_o$

$$T(E) = \left[1 + \left(\frac{k^2 - k_2^2}{2kk_2}\right)^2 \sin^2(k_2 L)\right]^{-1}$$

# Single Barrier - Key Summary

- Quantum wavefunctions can tunnel through barriers
- Tunneling is reduced with increasing barrier height and width

- Transmission above the barrier is not unity
  - »2 interfaces cause constructive and destructive interference
  - »Quasi bound states are formed that result in unity transmission

# Presentation Outline

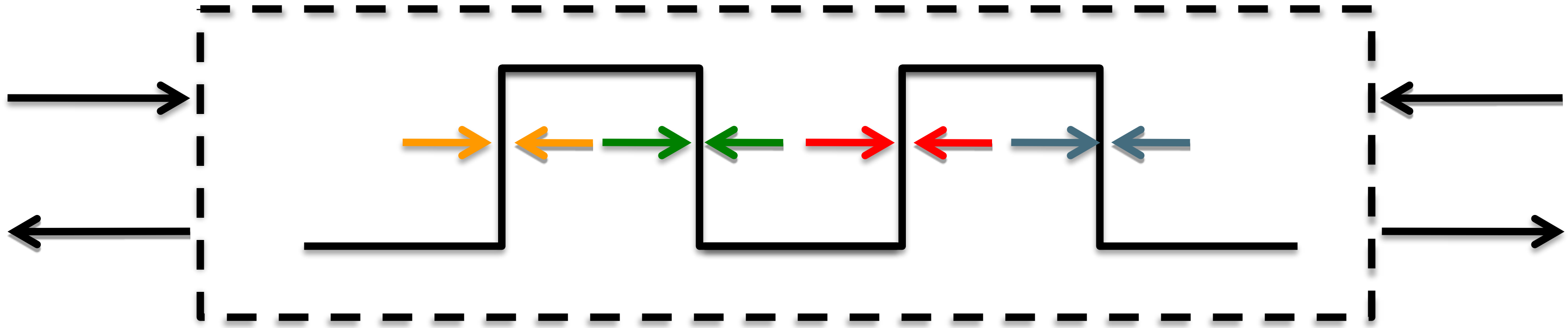
- Analytical solutions of Toy Problems
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers

**Reference:**

- piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt

# Double Barrier Transmission: Scattering Matrix approach

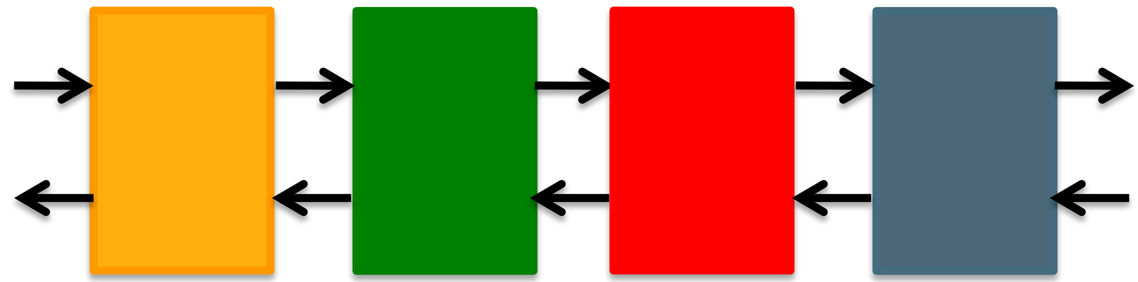
Define our system : Double barrier



One matrix each for each interface: 4 S-matrices

Left Incident

Reflected



Transmitted

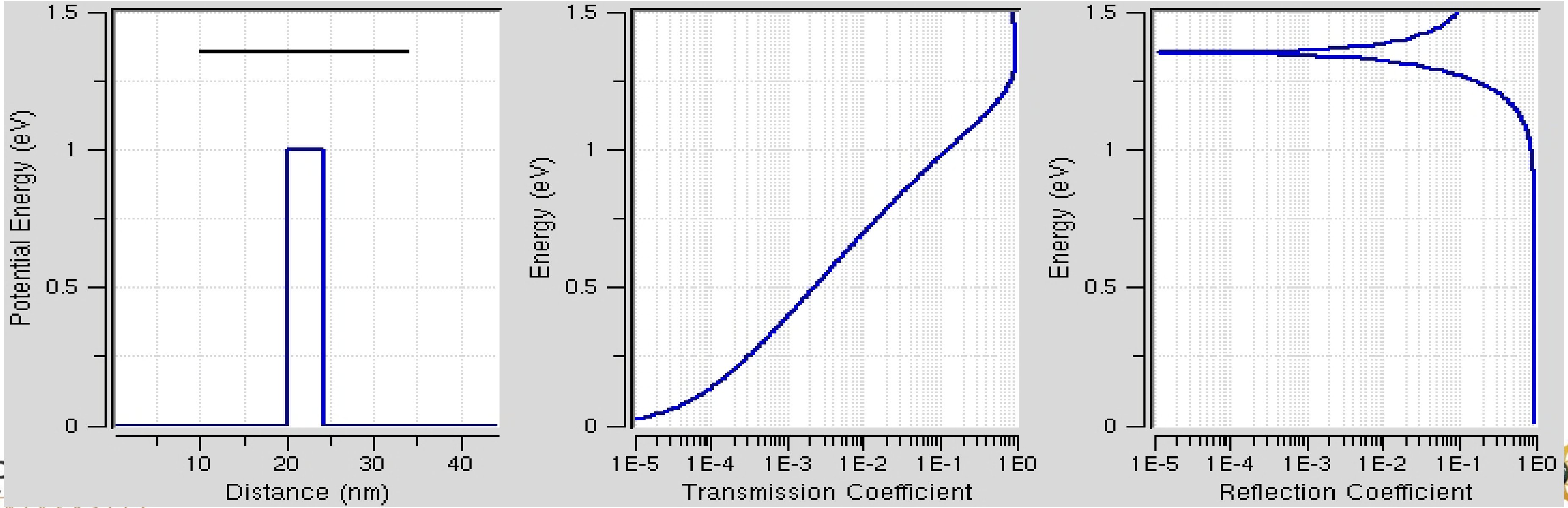
Right Incident

No particles lost!
Typically Left Incident wave is normalized to one.
Right incident is assumed to be zero.

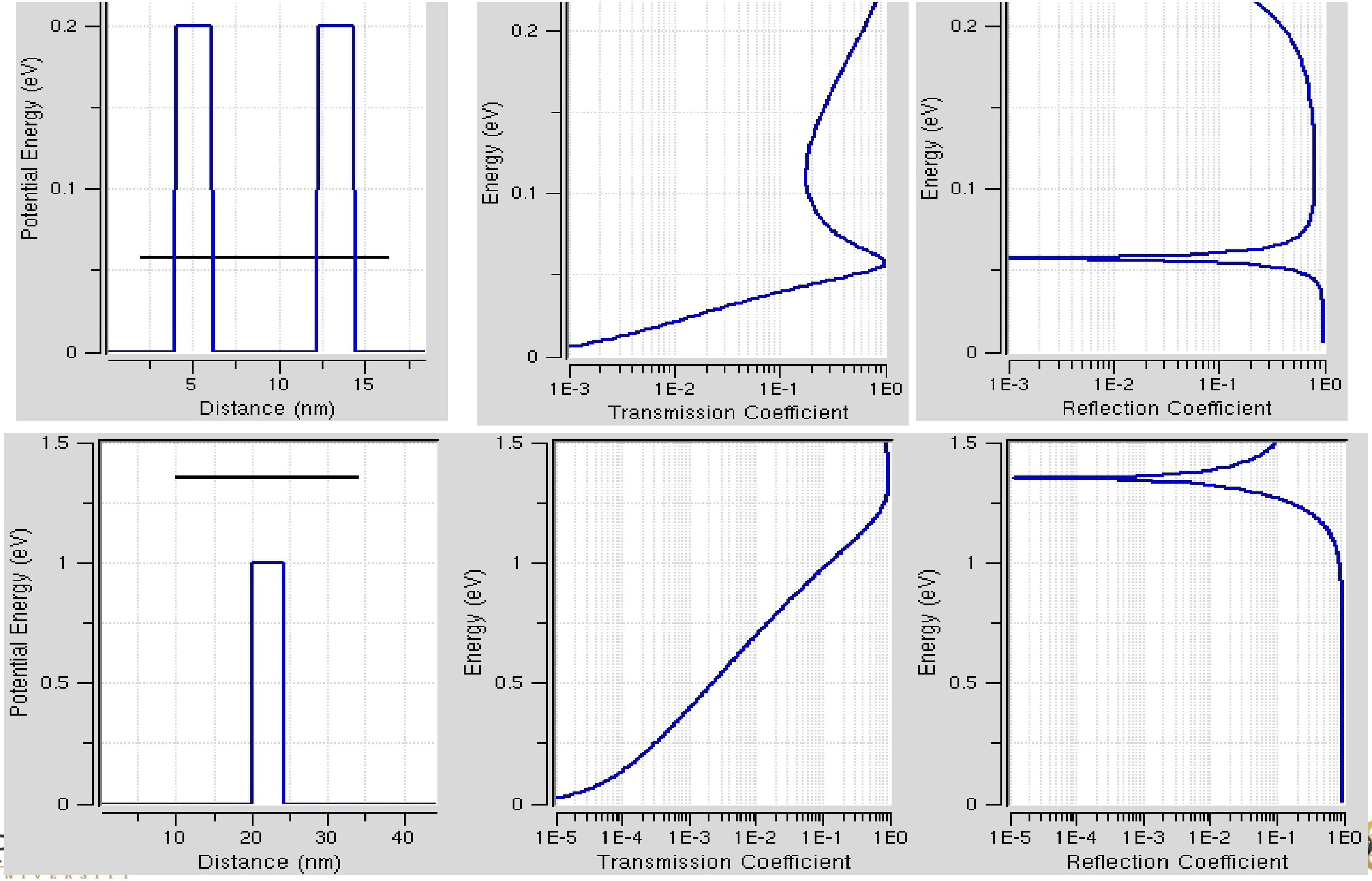
Also this problem is analytically solvable! => Homework assignment

# Reminder: Single barrier

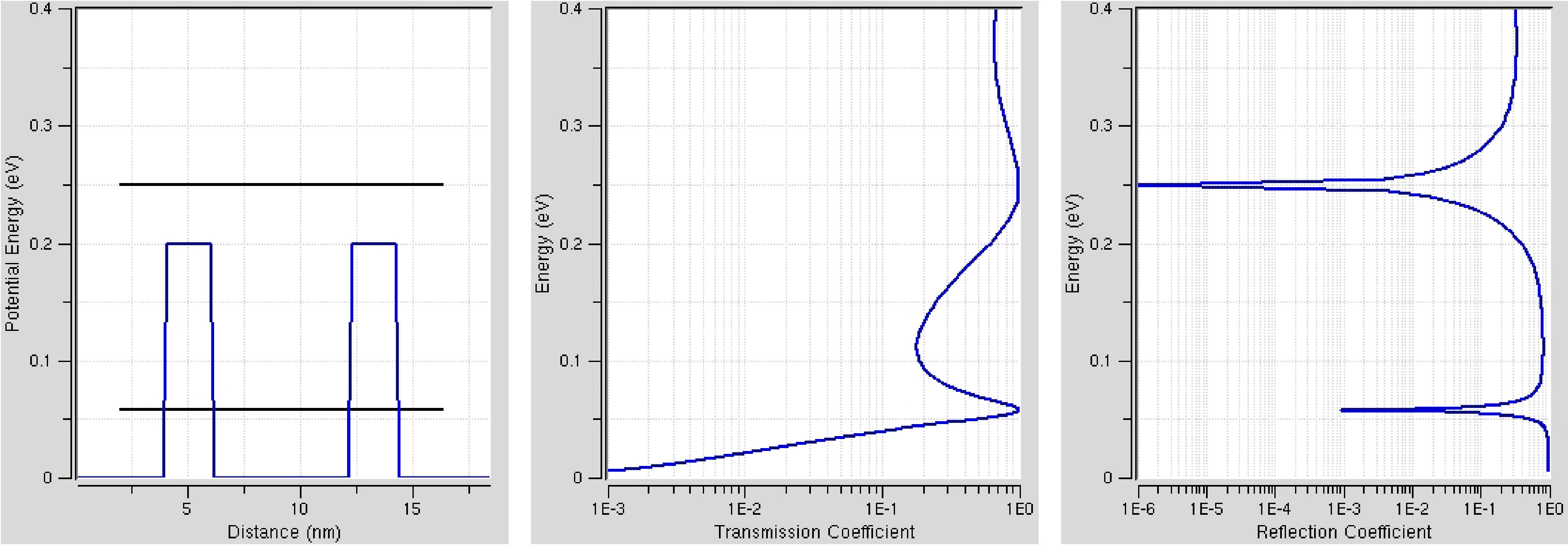
- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier.
  Transmission goes to one.



- Double barriers allow a transmission probability of one / unity for discrete energies
- (reflection probability of zero) for some energies below the barrier height.
- This is in sharp contrast to the single barrier case
- Cannot be predicted by classical physics.

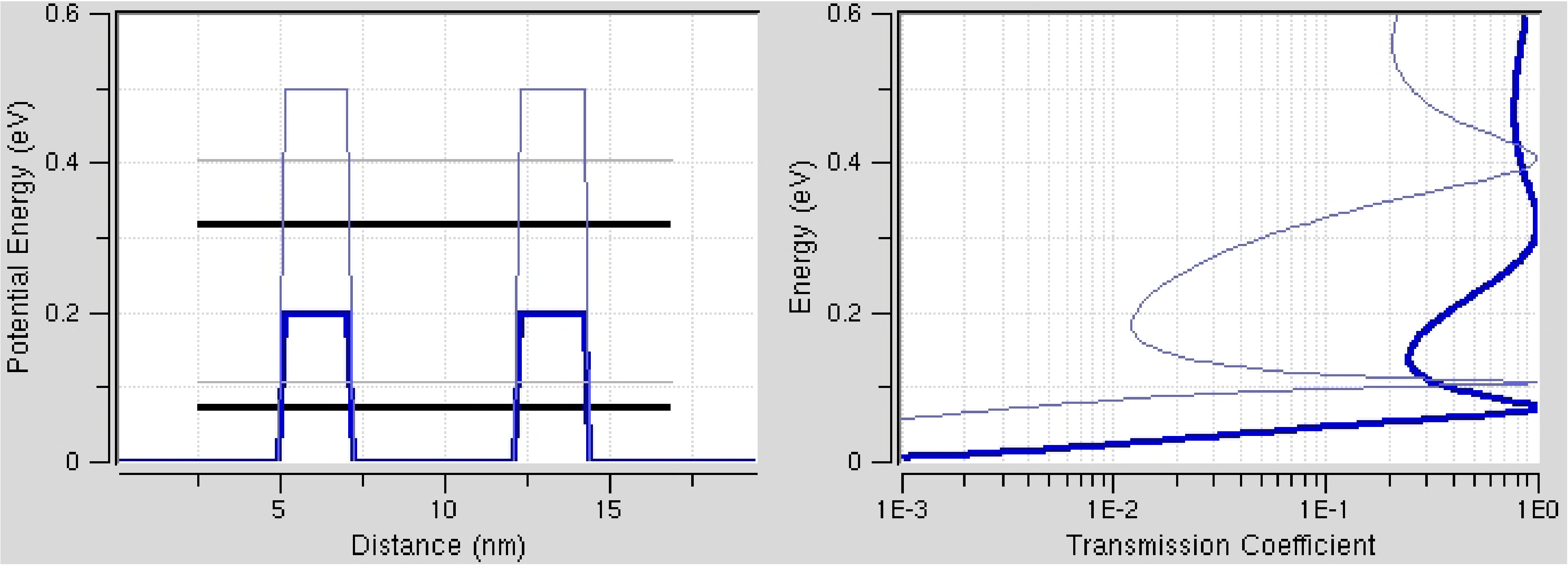


# Double barrier: Quasi-bound states



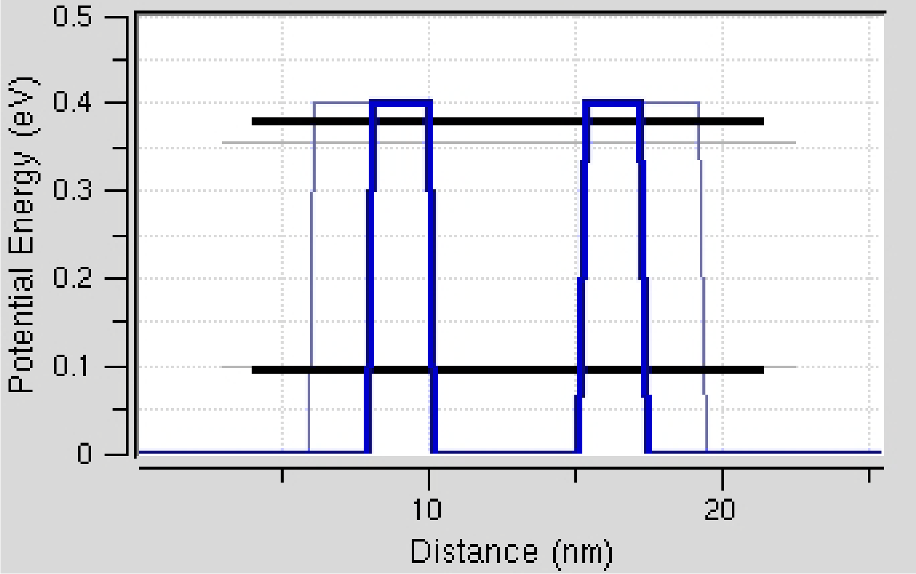

- In addition to states inside the well, there could be states above the barrier height.
- States above the barrier height are quasi-bound or weakly bound.
- How strongly bound a state is can be seen by the width of the transmission peak.
- The transmission peak of the quasi-bound state is much broader than the peak for the state inside the well.

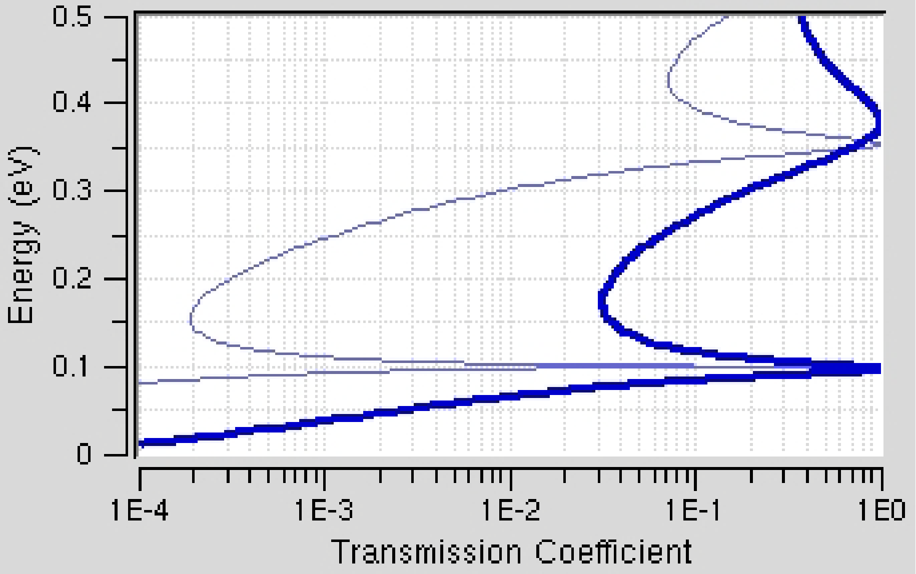
# Effect of barrier height




- Increasing the barrier height makes the resonance sharper.
- By increasing the barrier height, the confinement in the well is made stronger, increasing the lifetime of the resonance.
- A longer lifetime corresponds to a sharper resonance.

# Effect of barrier thickness

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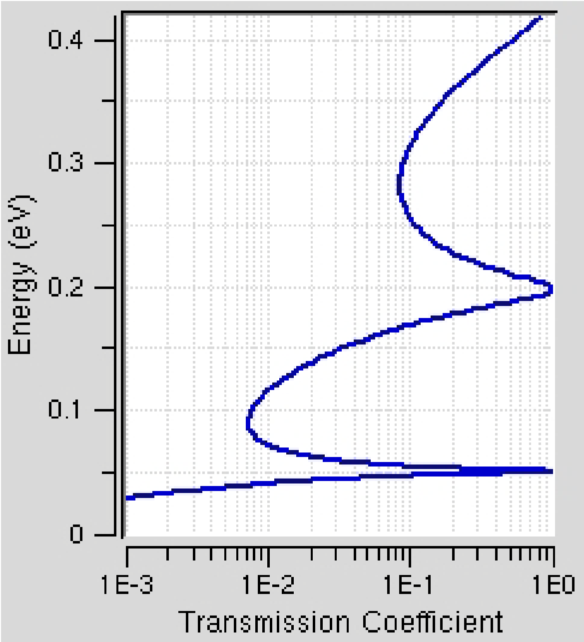
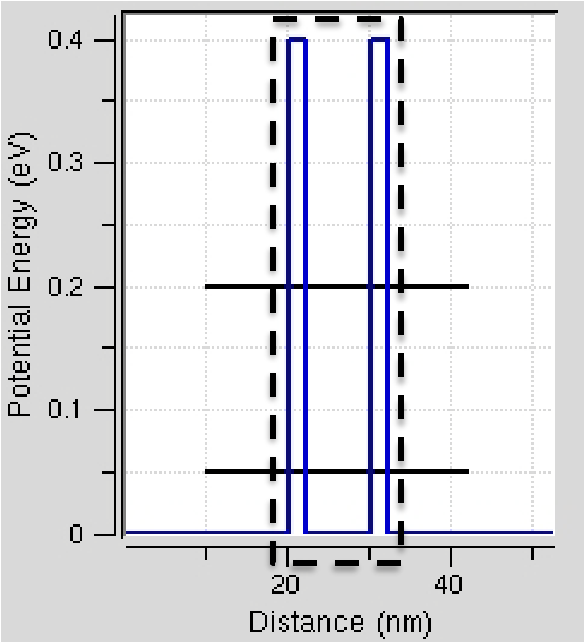
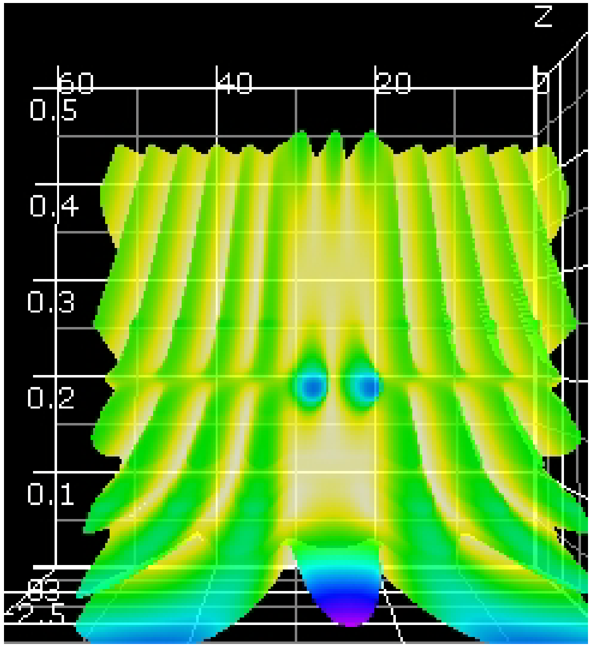
# Double barrier energy levels Vs Closed system




The well region in the double barrier case can be thought of as a particle in a box.

# Particle in a box

- The time independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \quad \text{where, } V(x) = \begin{cases} 0 & 0 < x < L_x \\ \infty & \text{elsewhere} \end{cases}$$

- The solution in the well is:

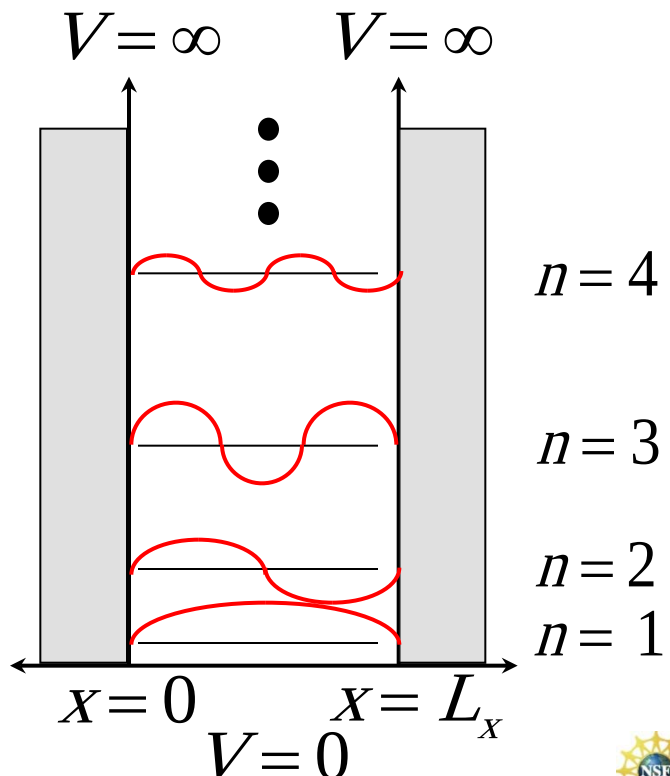
$$\psi_n(x) = A\sin\left(\frac{n\pi}{L_x}x\right), \quad n = 1, 2, 3, \ldots$$

- Plugging the normalized wave-functions back into the Schrödinger equation we find that energy levels are quantized.

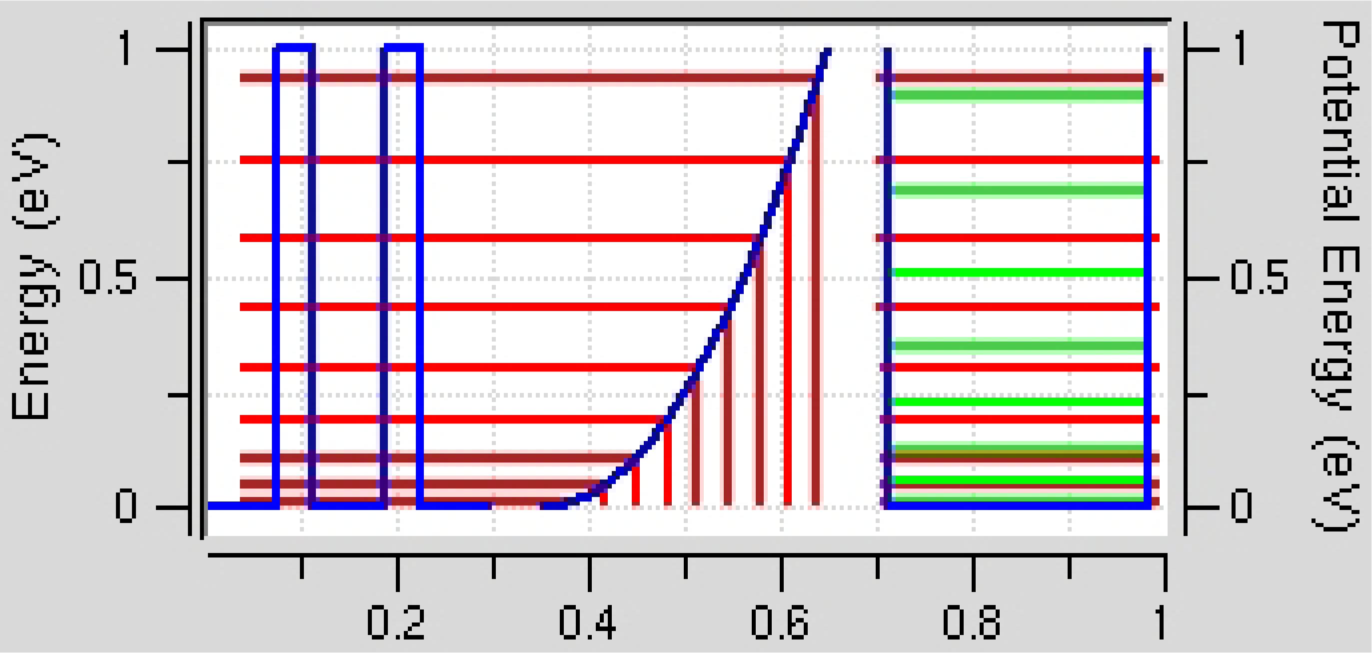
$$\psi_n(x) = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right)$$

$$E_n = \frac{h^2\pi^2}{2mL_x^2}n^2$$

$$n = 1, 2, 3, \ldots, \quad 0 < x < L_x$$



# Double barrier & particle in a box




- Green: Particle in a box energies.
- Red: Double barrier energies

- Double barrier: Thick Barriers(10nm), Tall Barriers(1eV), Well(20nm).
- First few resonance energies match well with the particle in a box energies.
- The well region resembles the particle in a box setup.

# Open systems Vs closed systems

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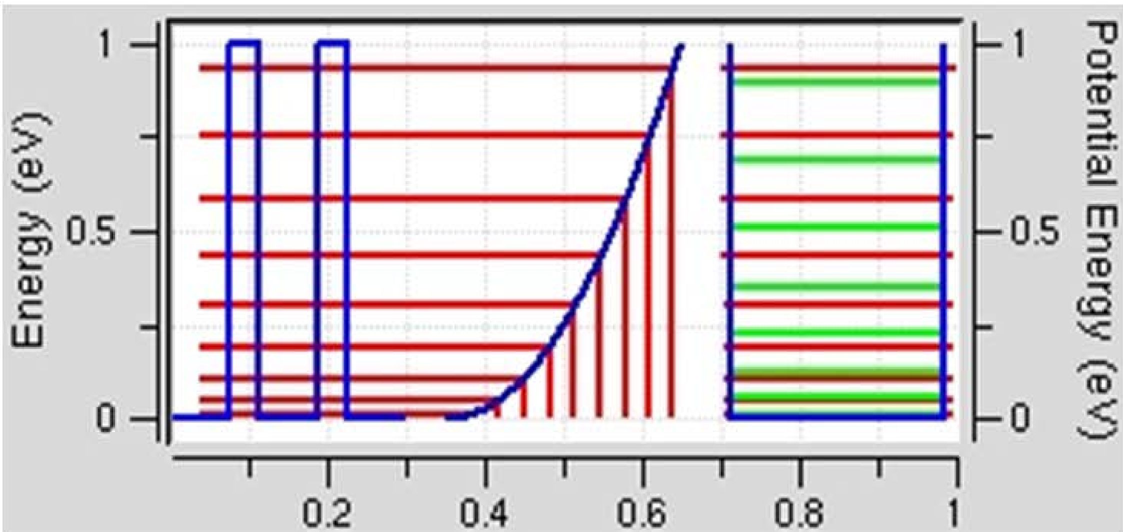
## Double barrier & particle in a box

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- First few resonance energies match well with the particle in a box energies.
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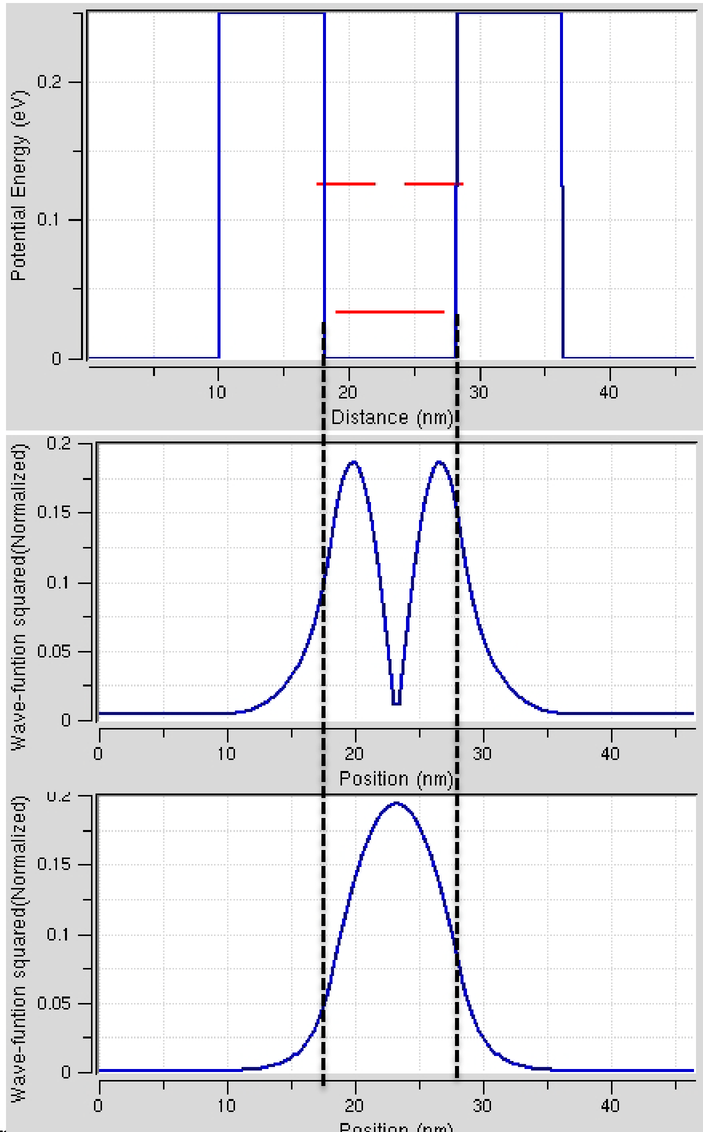
PURDUE UNIVERSITY Klimeck – ECE606 Spring 2010 – notes adopted from Alam

# Reason for deviation?

Potential profile and resonance energies using tight-binding.

First excited state wave-function amplitude using tight binding.

Ground state wave-function amplitude using tight binding.




- Wave-function penetrates into the barrier region.
- The effective length of the well region is modified.
- The effective length of the well is crucial in determining the energy levels in the closed system.

$$E_n = \frac{\hbar^2 \pi^2}{2 m L_{well}^2} n^2$$

$$n = 1, 2, 3, \ldots, \quad 0 < x < L_{well}$$

# Double Barrier Structures - Key Summary

- Double barrier structures can show unity transmission for energies BELOW the barrier height
  - » Resonant Tunneling
- Resonance can be associated with a quasi bound state
  - » Can relate the bound state to a particle in a box
  - » State has a finite lifetime / resonance width
- Increasing barrier heights and widths:
  - » Increases resonance lifetime / electron residence time
  - » Sharpens the resonance width

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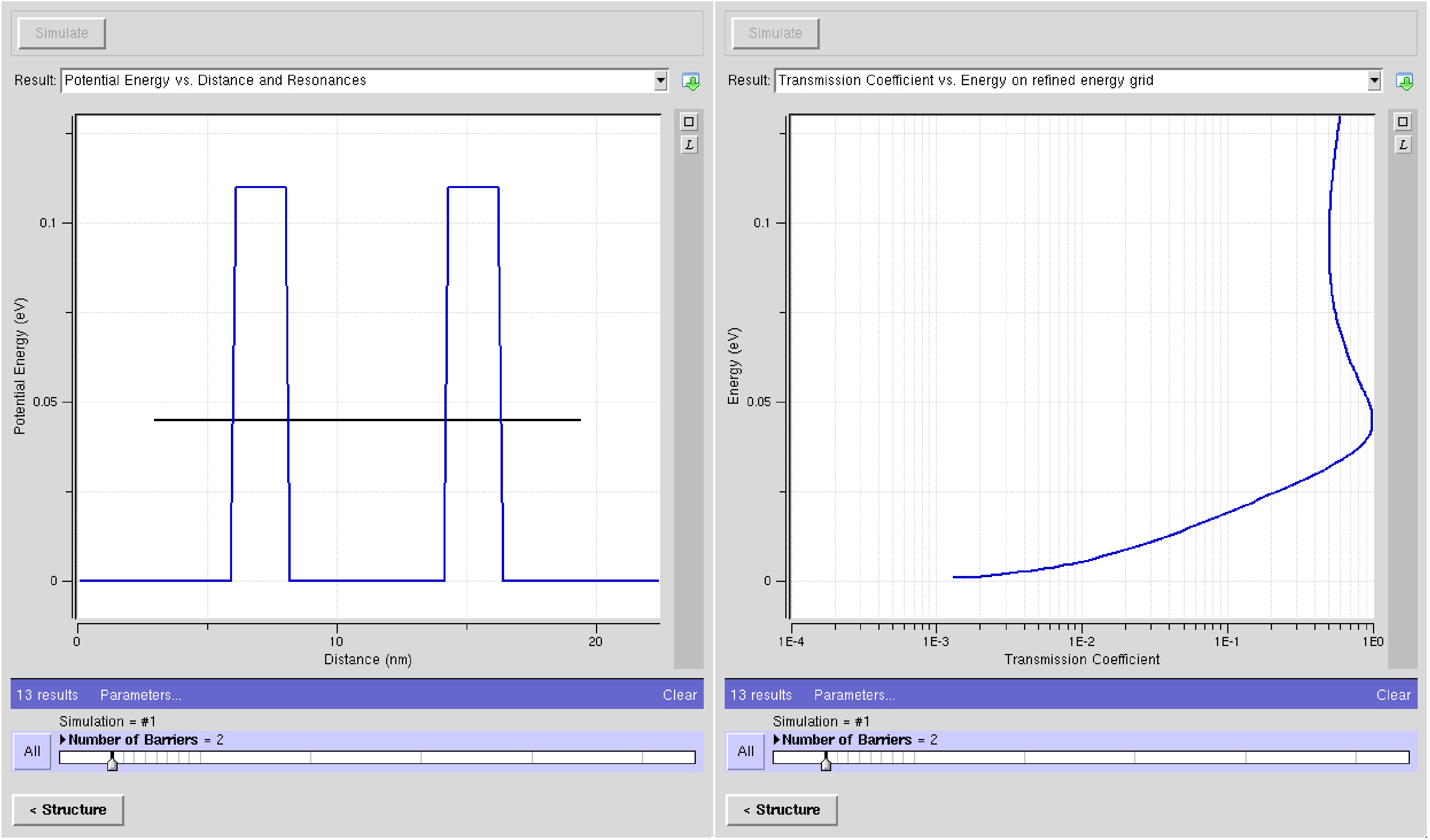
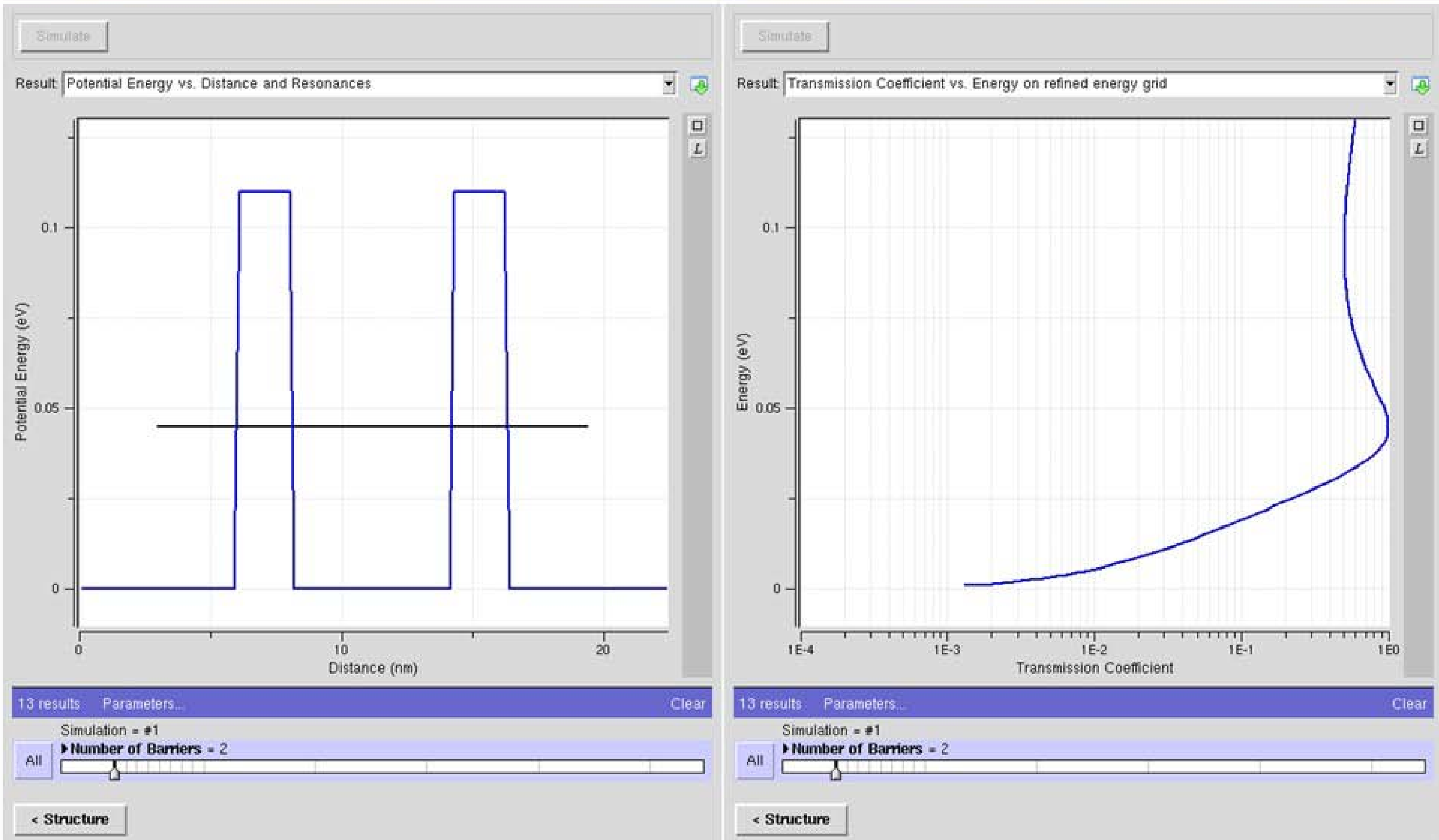
# 1 Well => 1 Transmission Peak




- Vb=110meV, W=6nm, B=2nm

# 2 Wells => 2 Transmission Peaks

# 1 Well => 1 Transmission Peak




- Vb=110meV, W=6nm, B=2nm



- Vb=110meV, W=6nm, B=2nm

Bonding/Anti-bonding State

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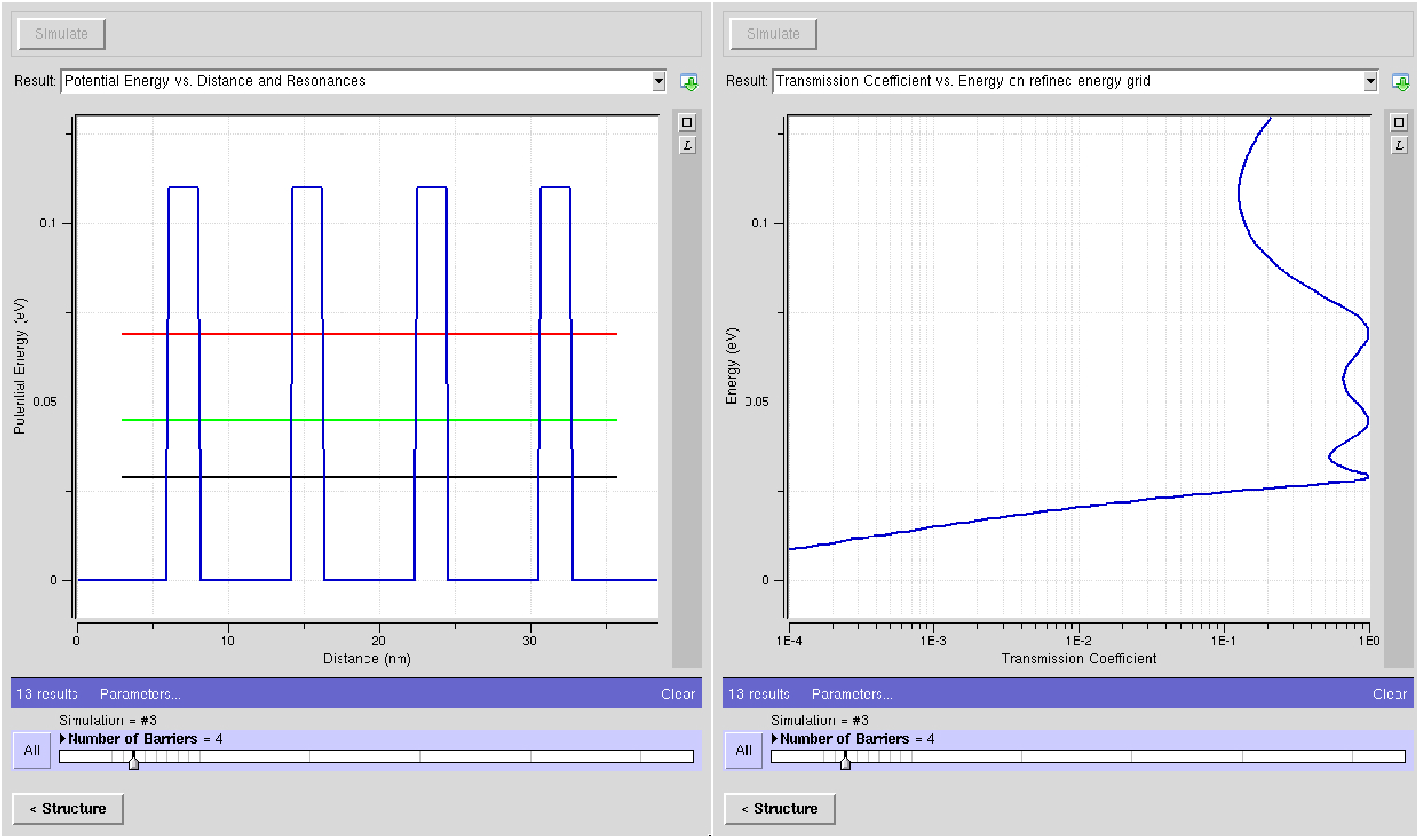
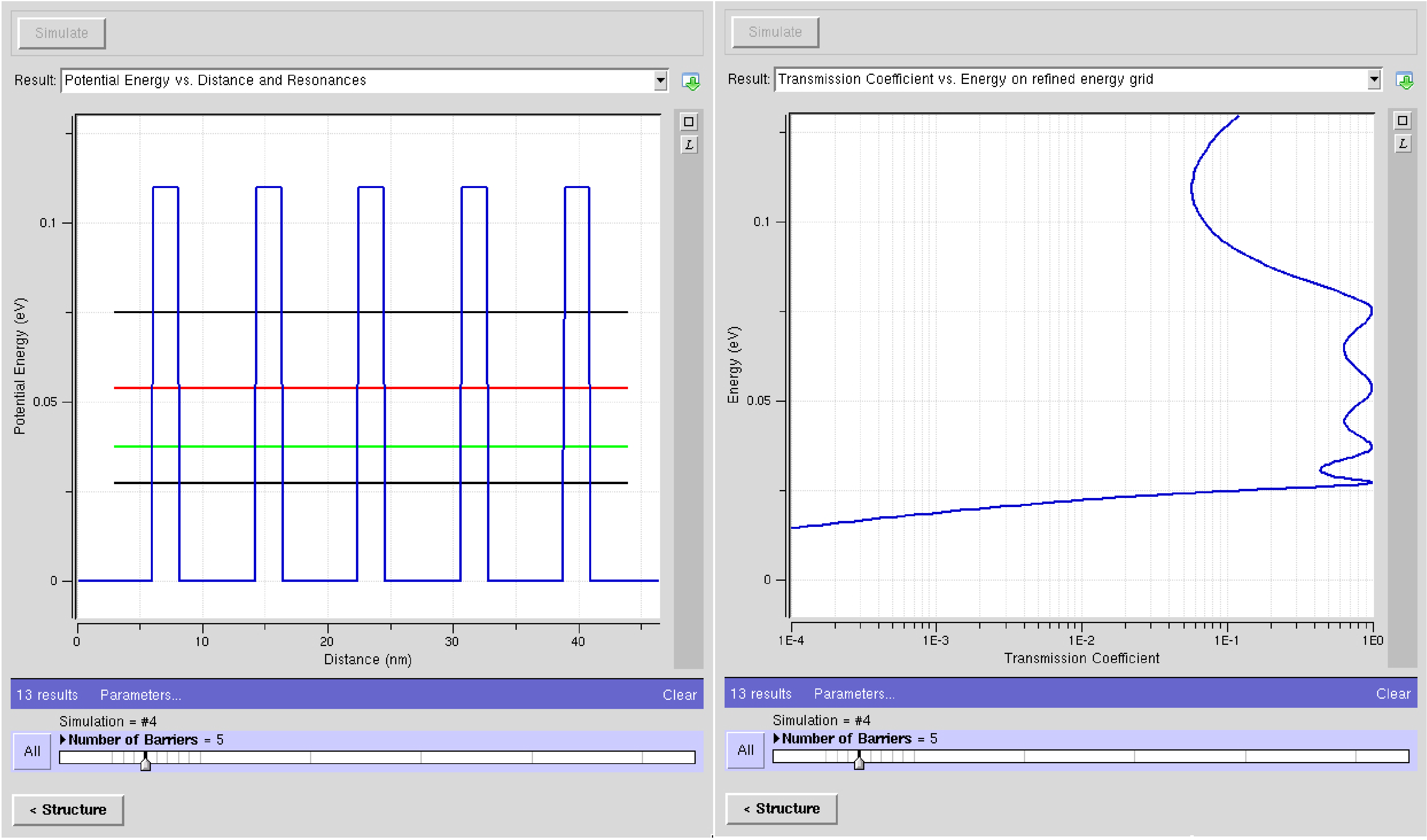
# 3 Wells => 3 Transmission Peaks



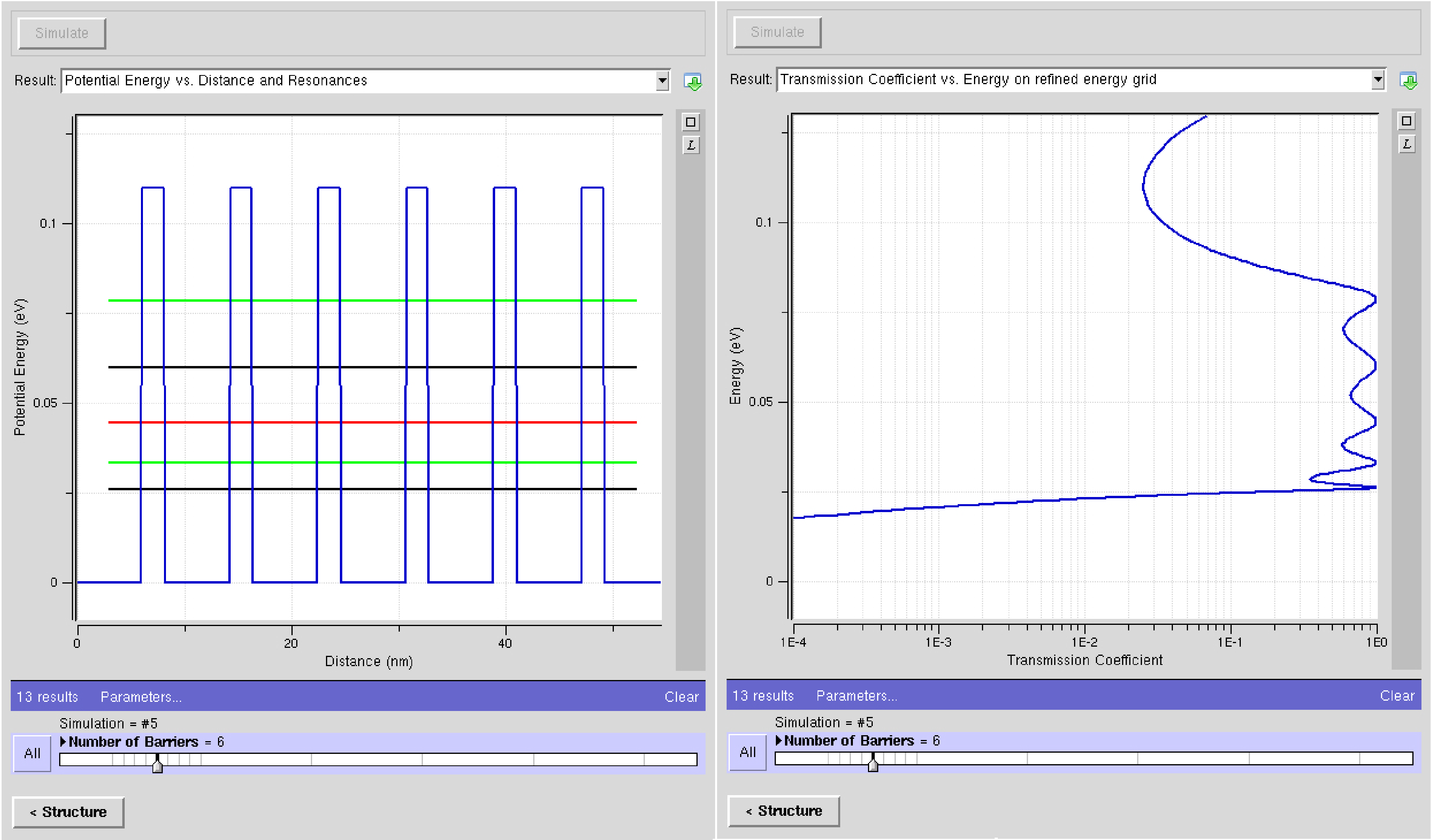

- Vb=110meV, W=6nm, B=2nm

# 4 Wells => 4 Transmission Peaks



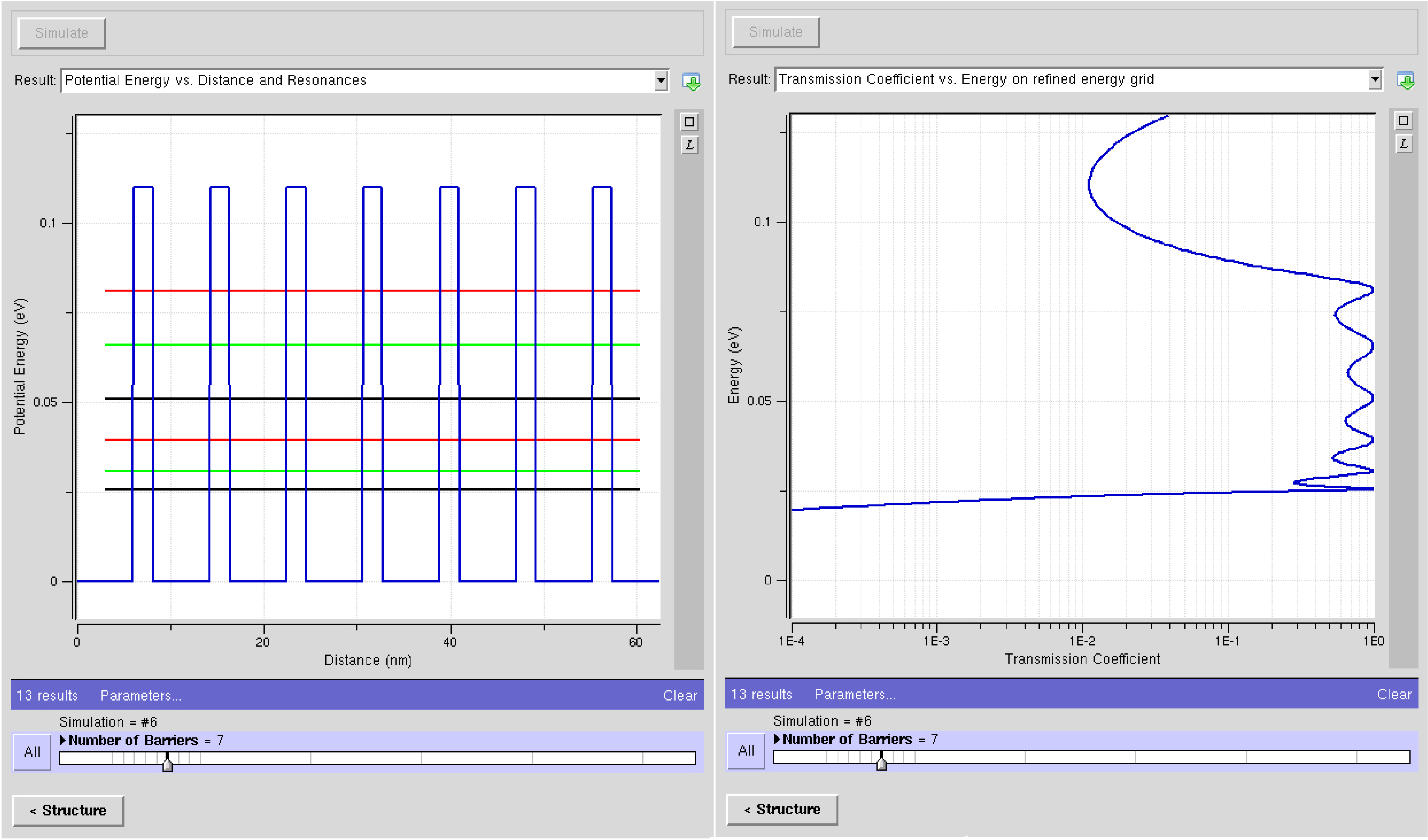

- Vb=110meV, W=6nm, B=2nm

# 5 Wells => 5 Transmission Peaks



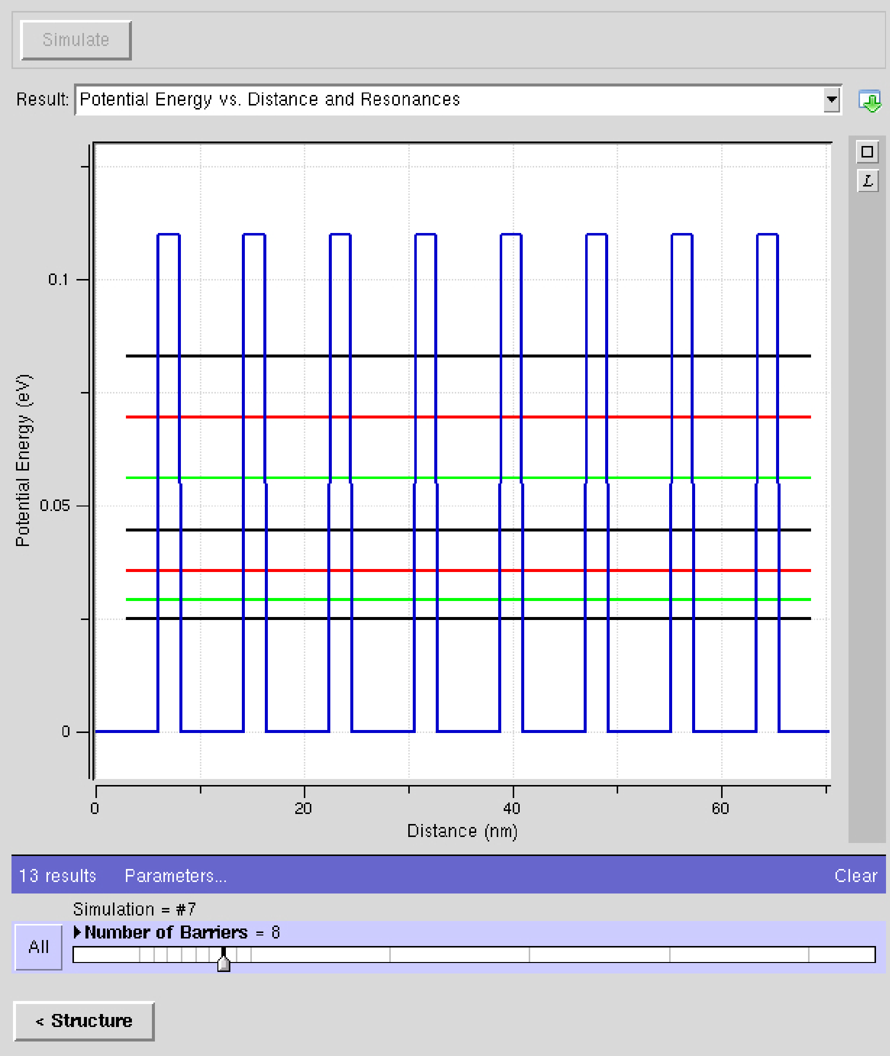

- Vb=110meV, W=6nm, B=2nm

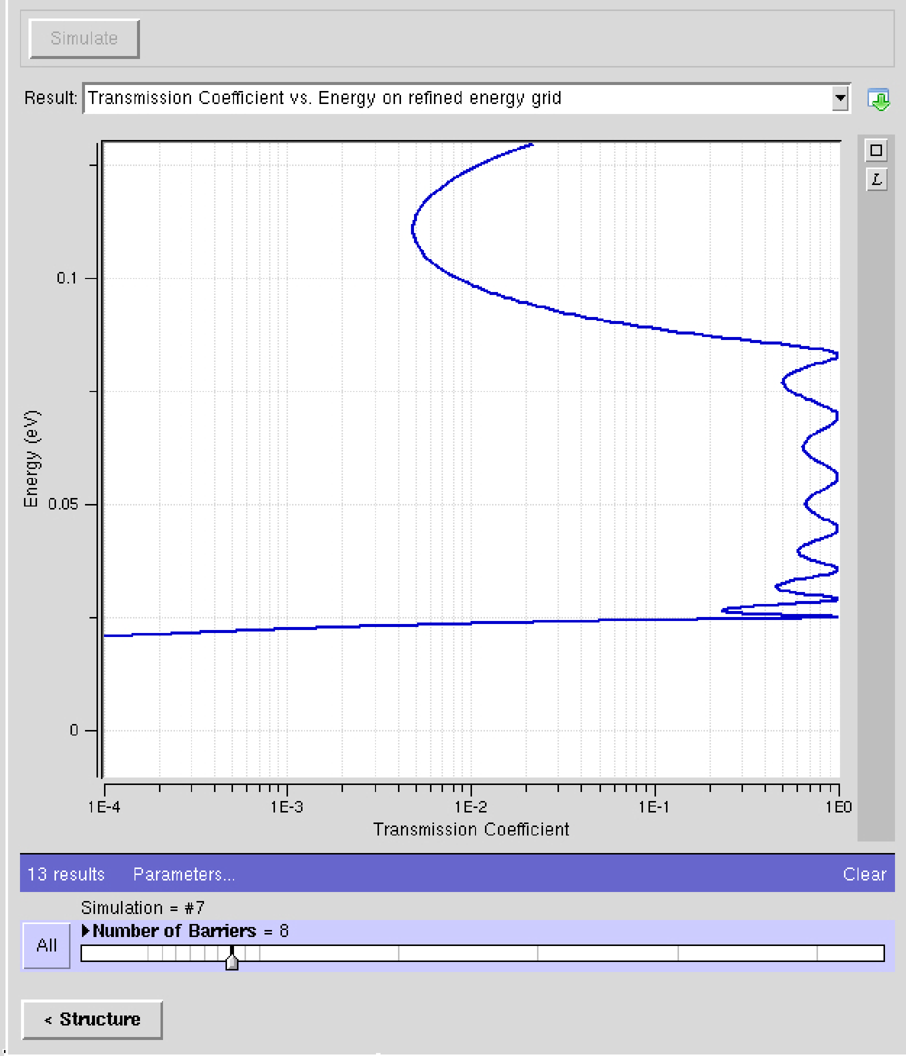
# 6 Wells => 6 Transmission Peaks




- Vb=110meV, W=6nm, B=2nm

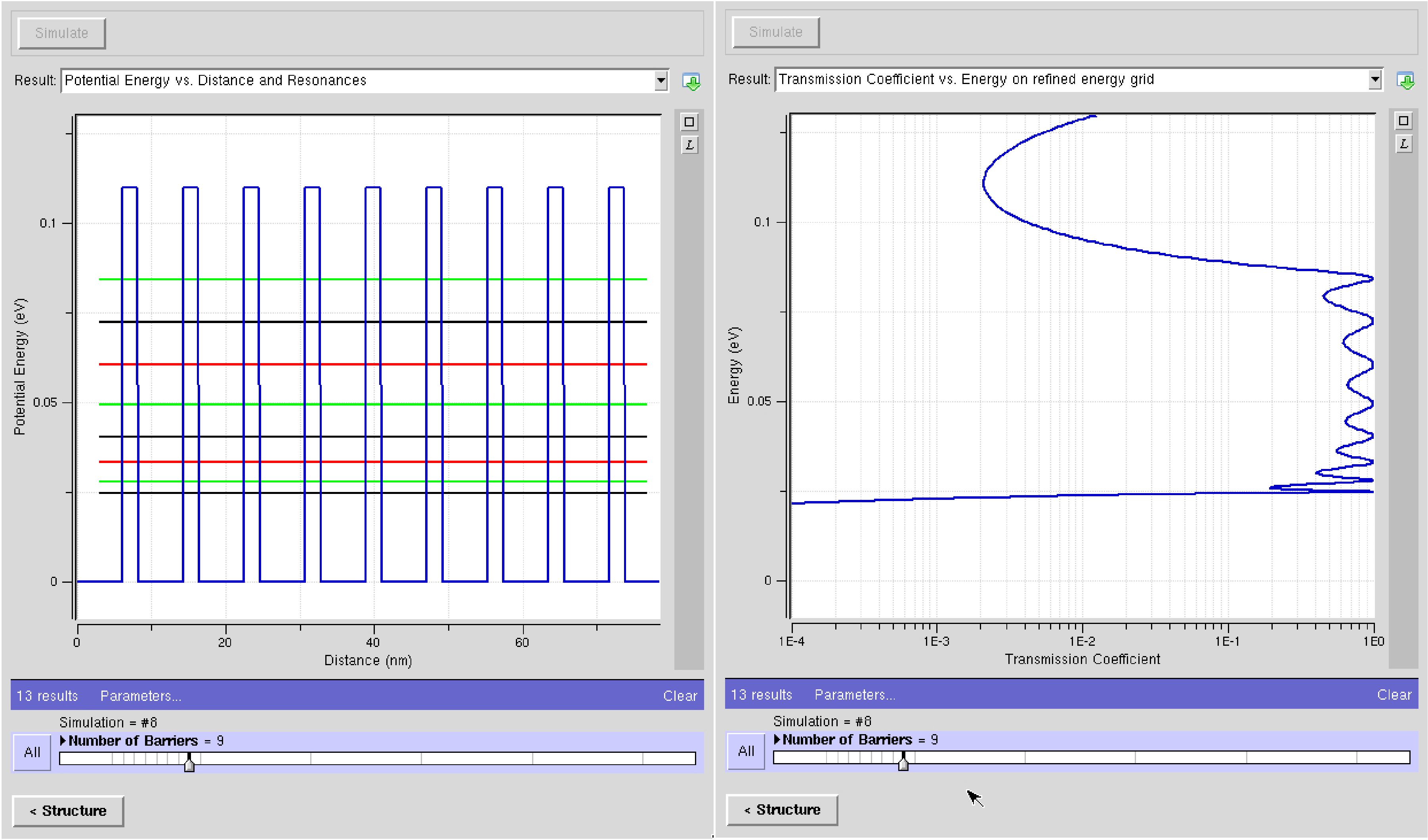
# 7 Wells => 7 Transmission Peaks



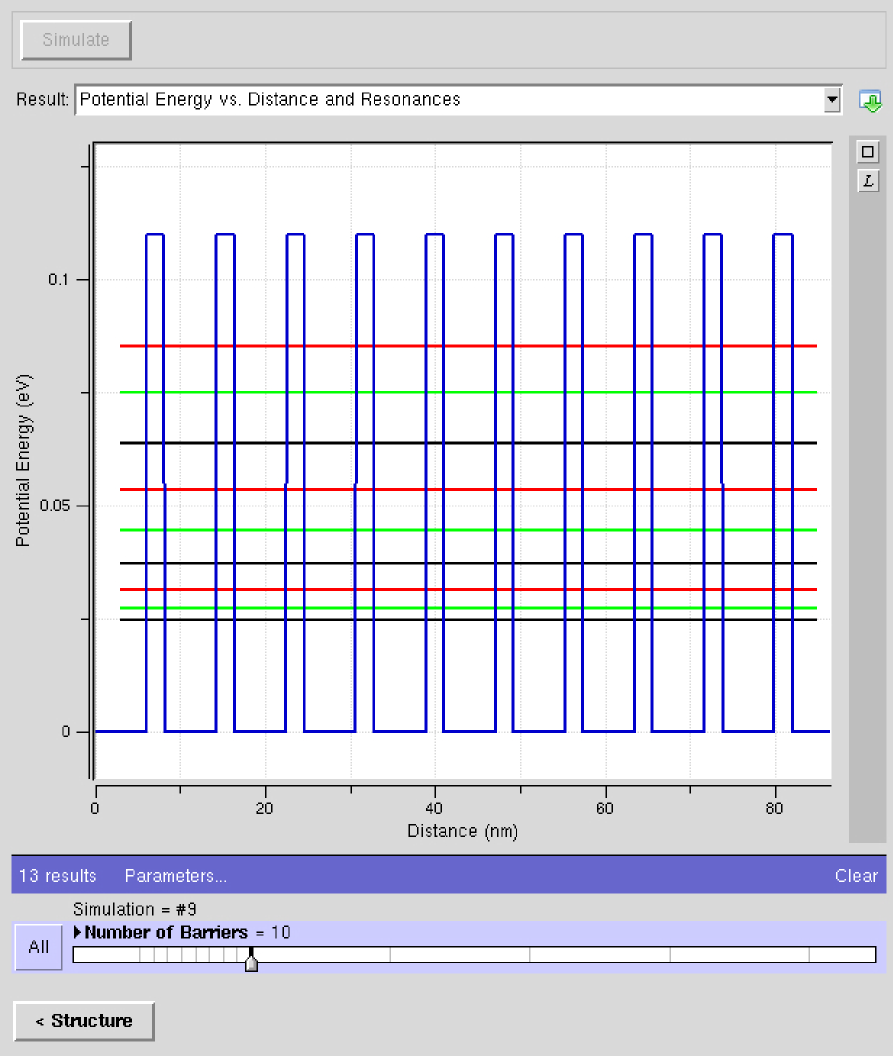

- Vb=110meV, W=6nm, B=2nm

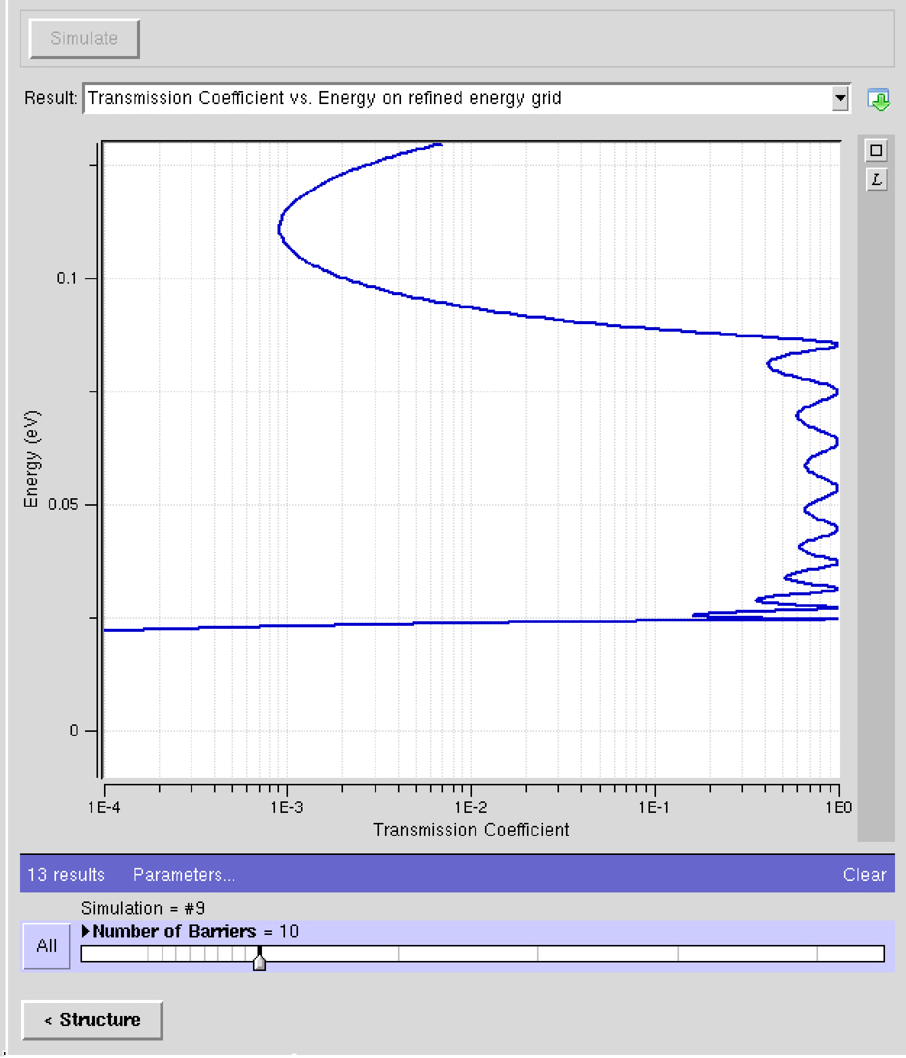
# 8 Wells => 8 Transmission Peaks




- Vb=110meV, W=6nm, B=2nm

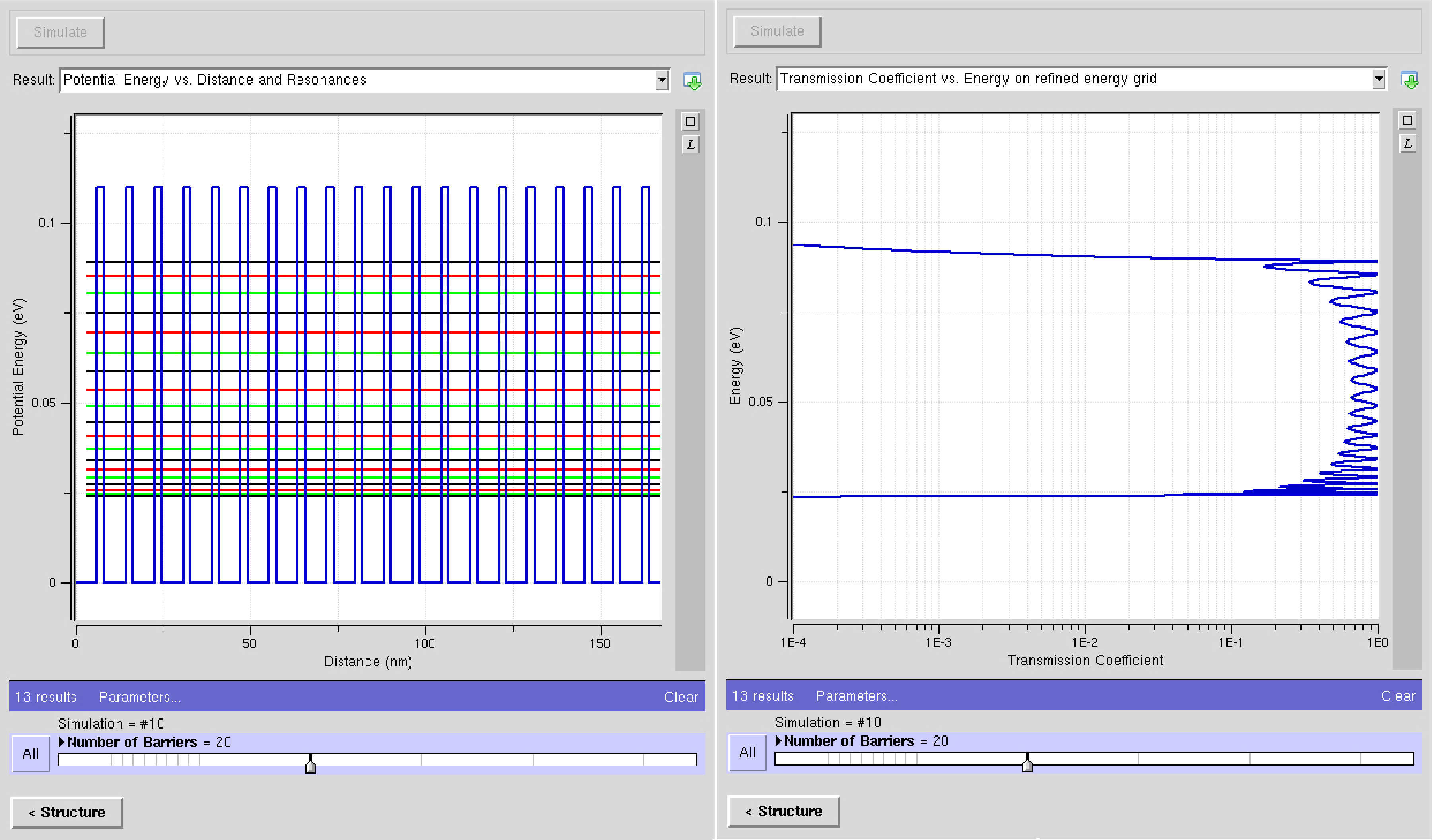
# 9 Wells => 9 Transmission Peaks




- Bandpass filter formed
- Band transmission not symmetric

# 19 Wells => 19 Transmission Peaks




- Bandpass filter formed
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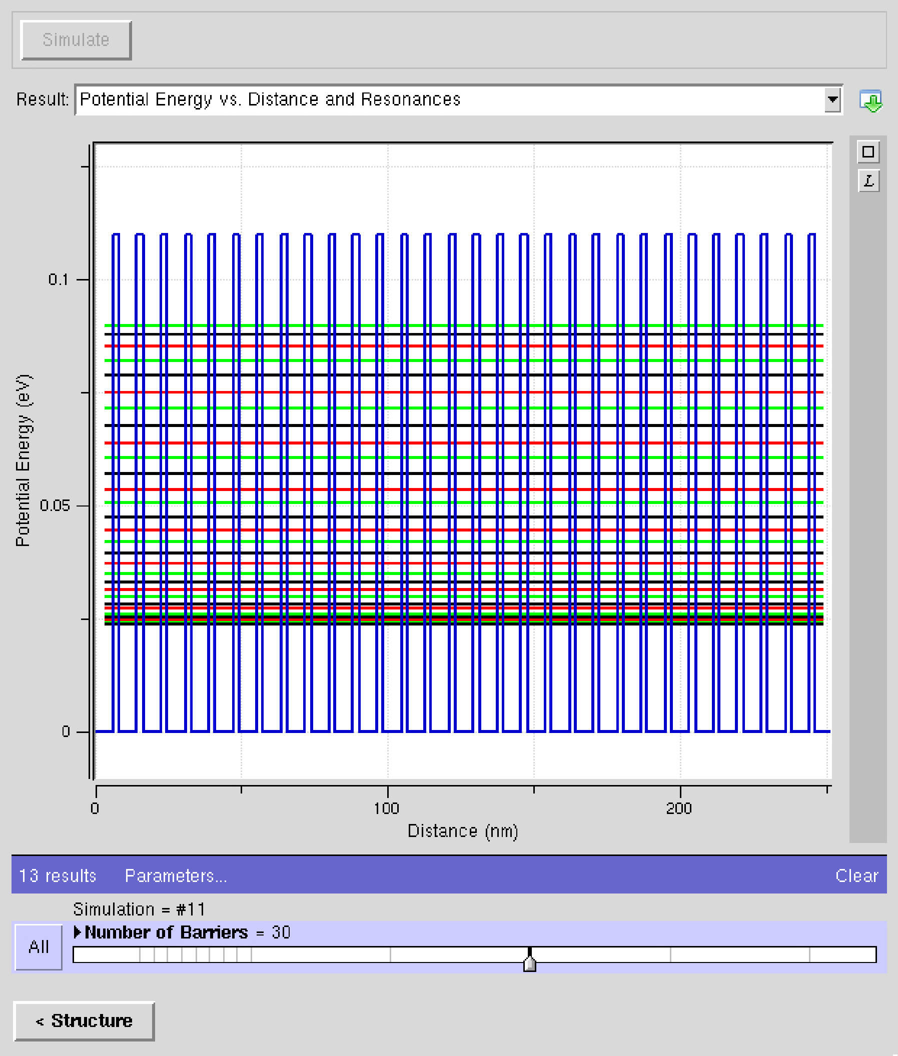
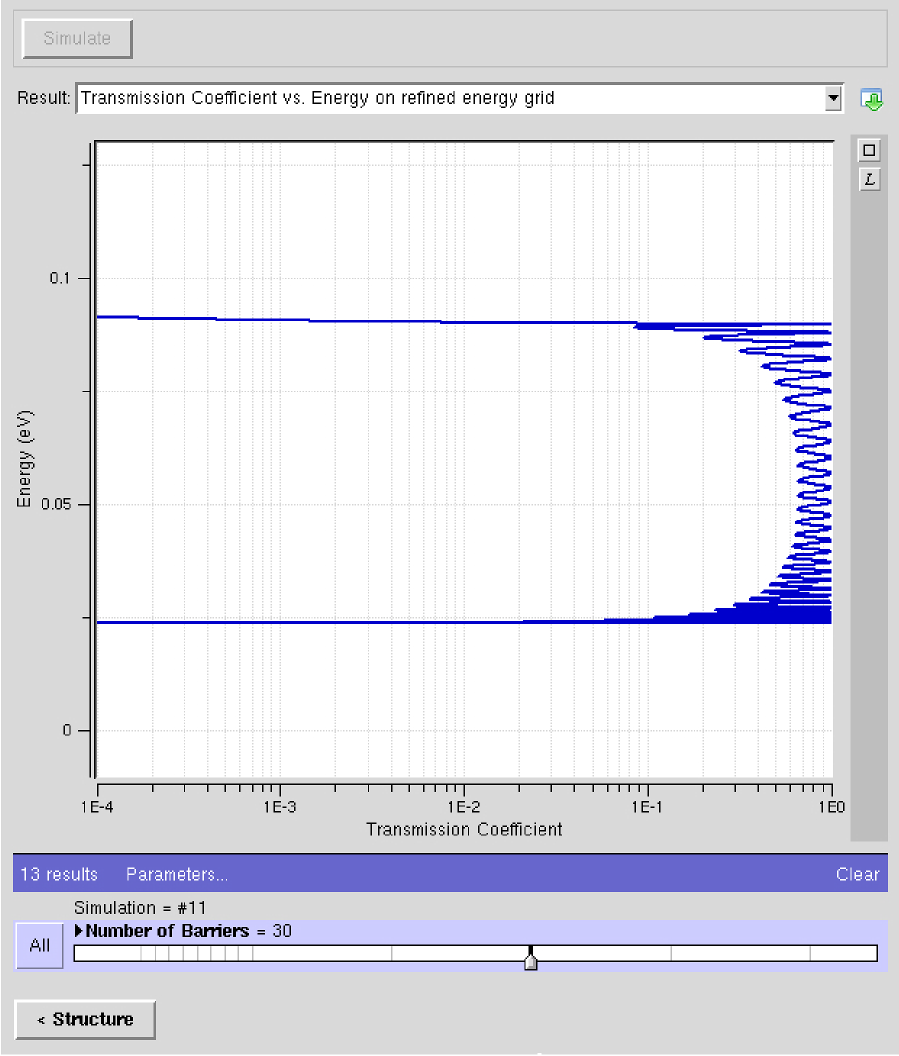
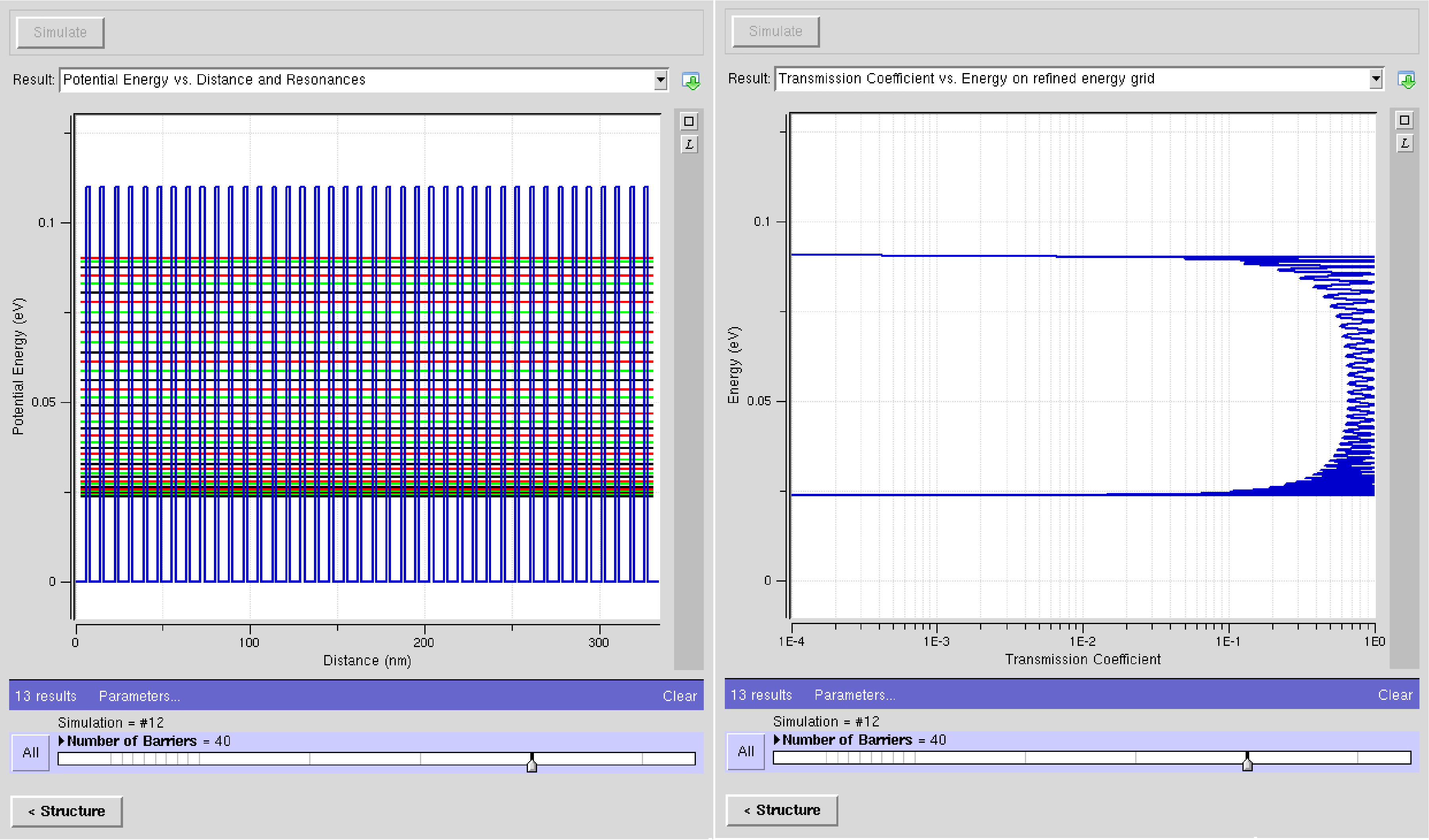
# 29 Wells => 29 Transmission Peaks



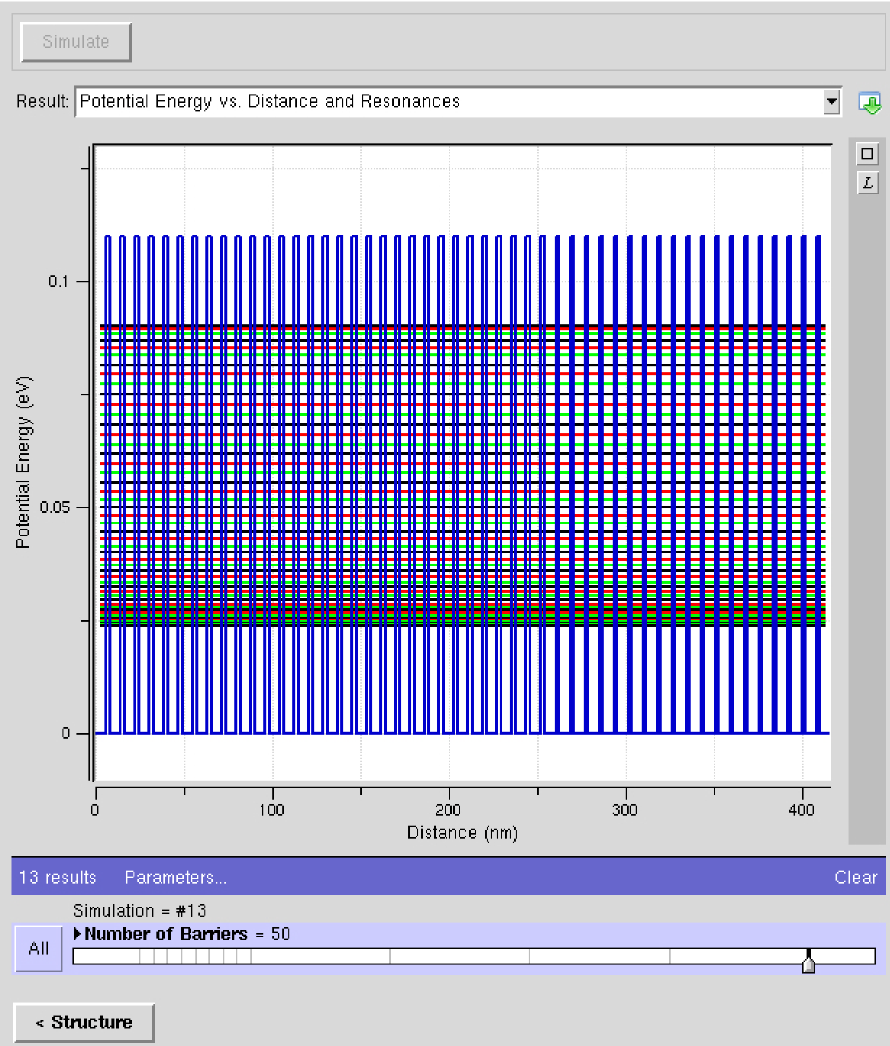

- Bandpass filter formed
- Band transmission not symmetric

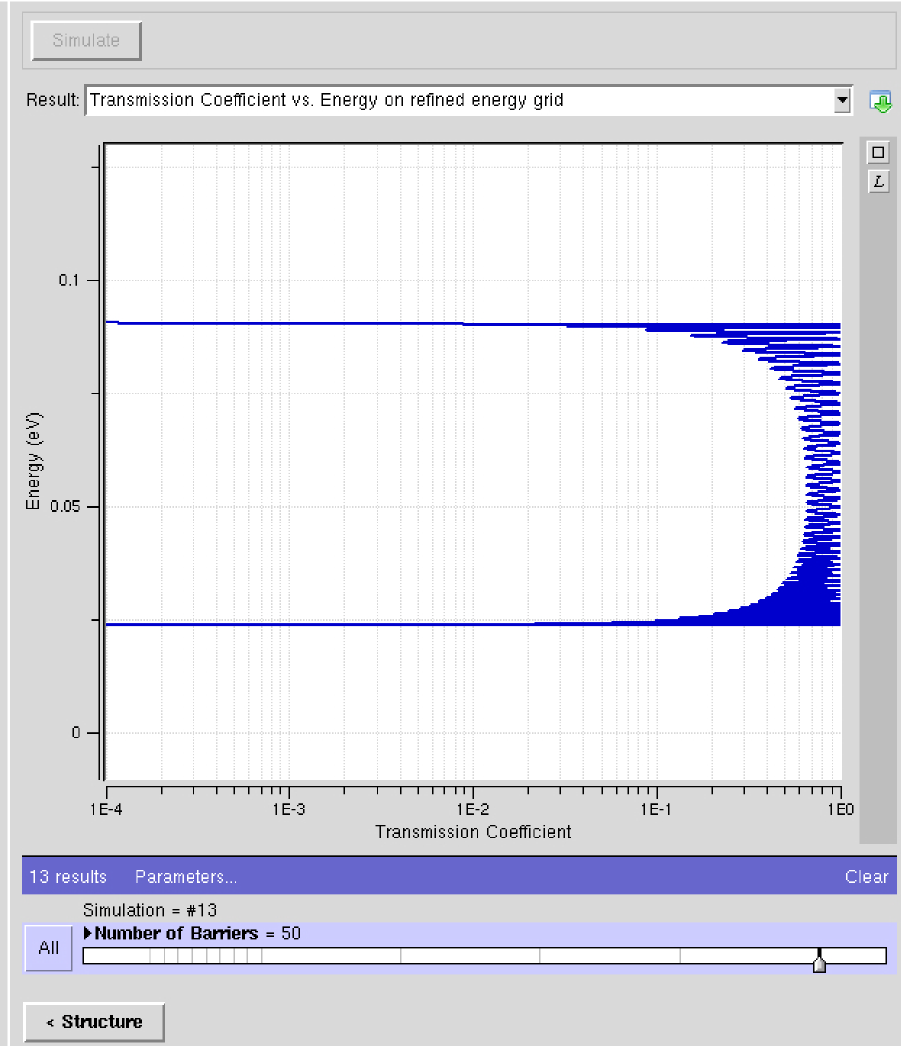
# 39 Wells => 39 Transmission Peaks




- Bandpass filter formed
- Band transmission not symmetric

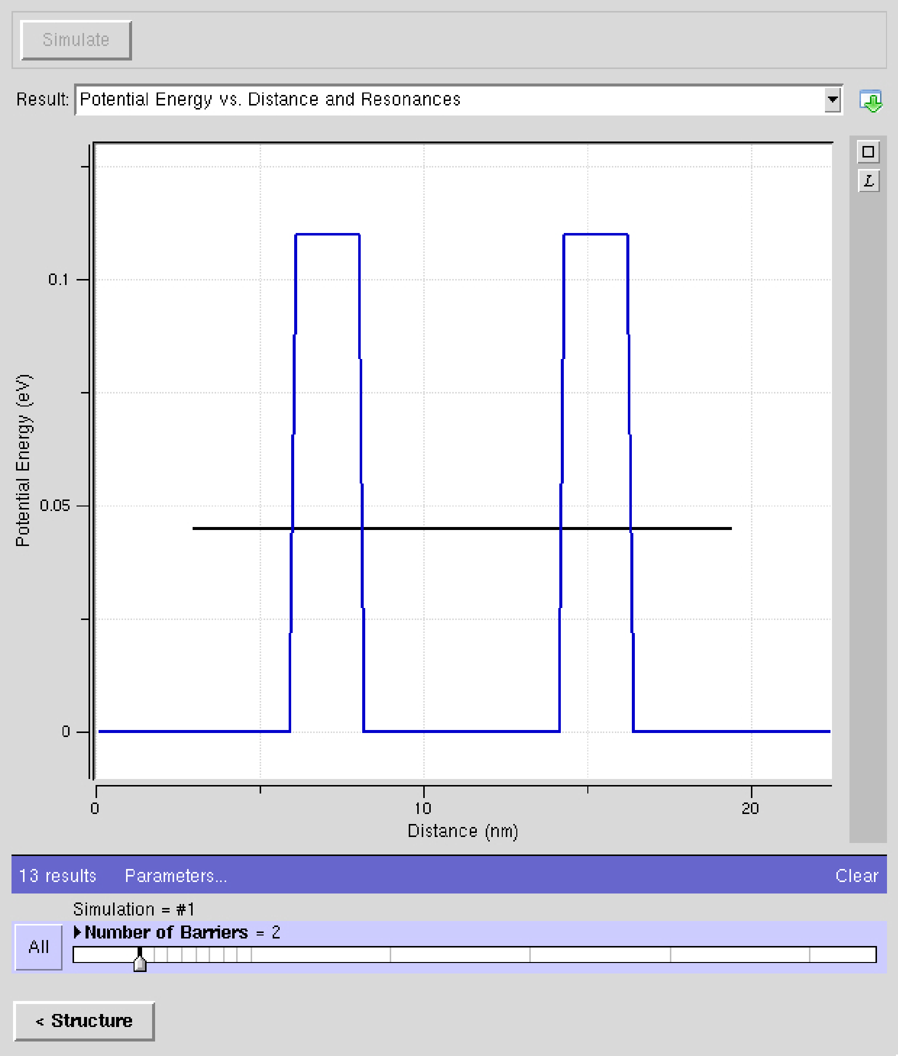
# 49 Wells => 49 Transmission Peaks

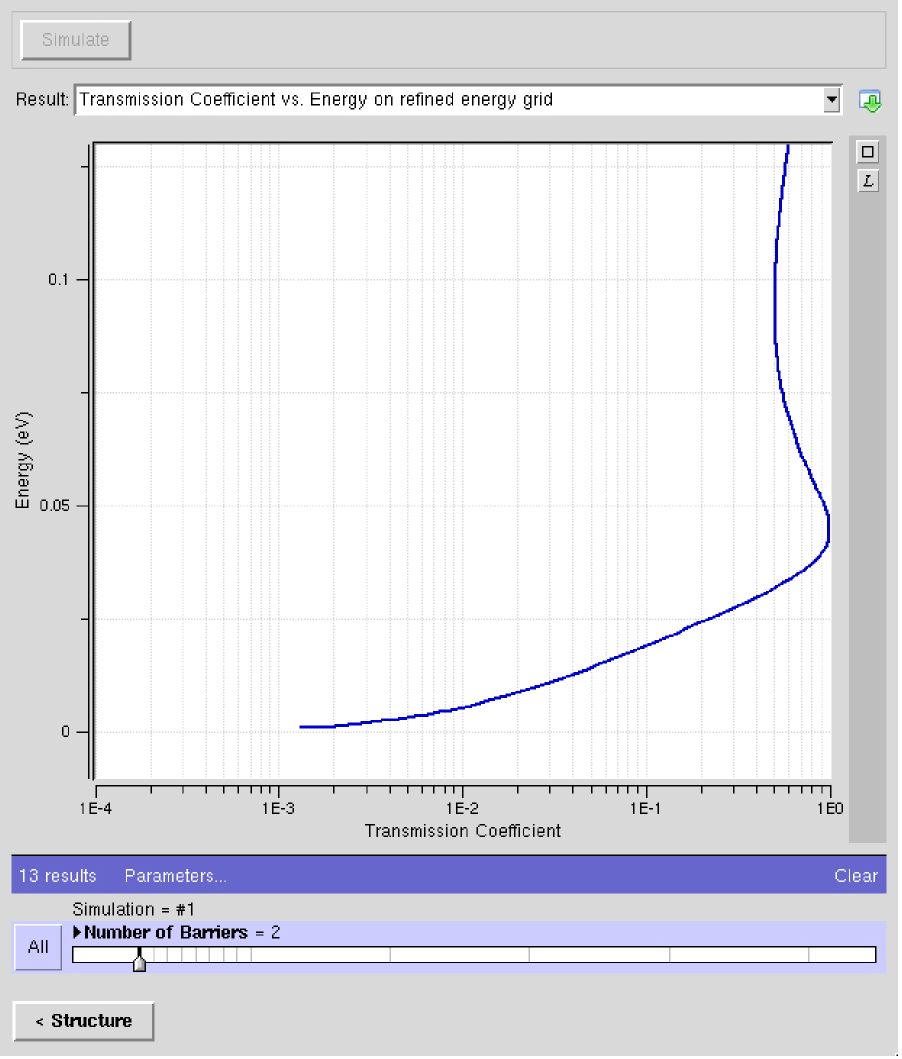



- Bandpass filter formed
- Band transmission not symmetric

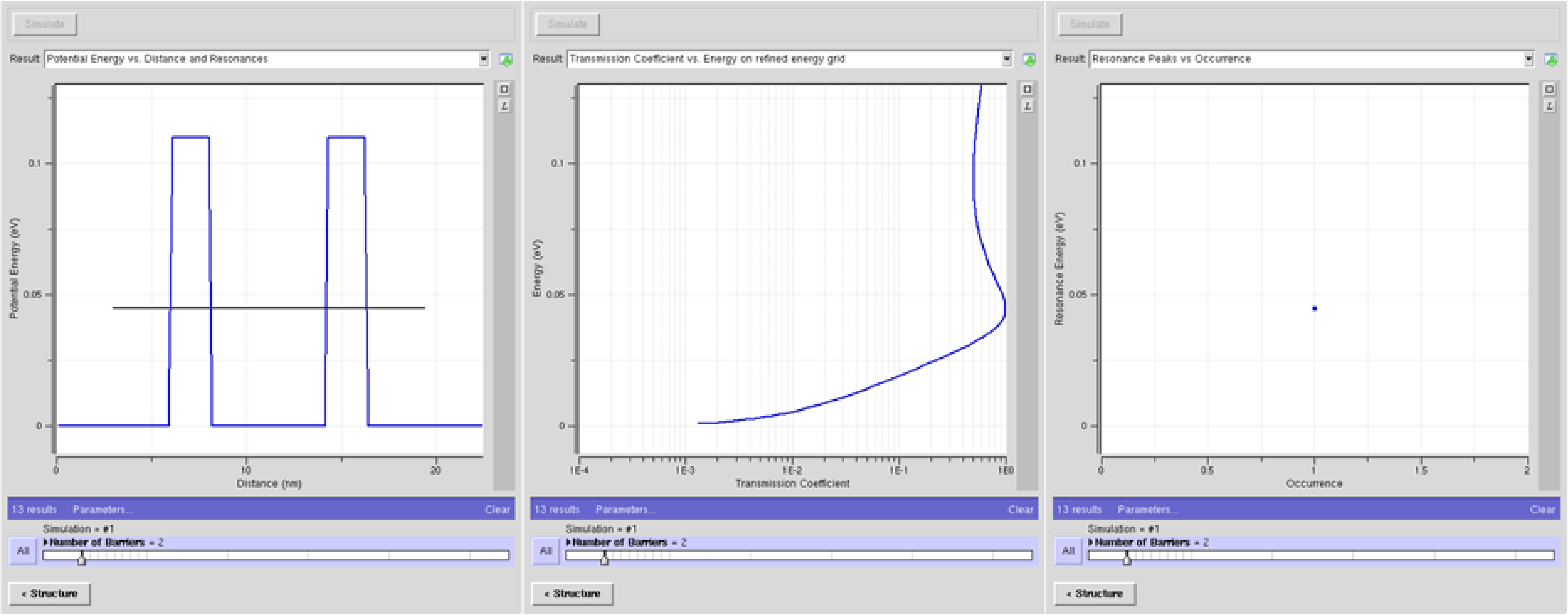
# N Wells => N Transmission Peaks




- Bandpass filter formed
- Band transmission not symmetric
- Bandpass sharpens with increasing number of wells

# 1 Well => 1 Transmission Peak => 1 State




- Bandpass filter formed
- Band transmission not symmetric
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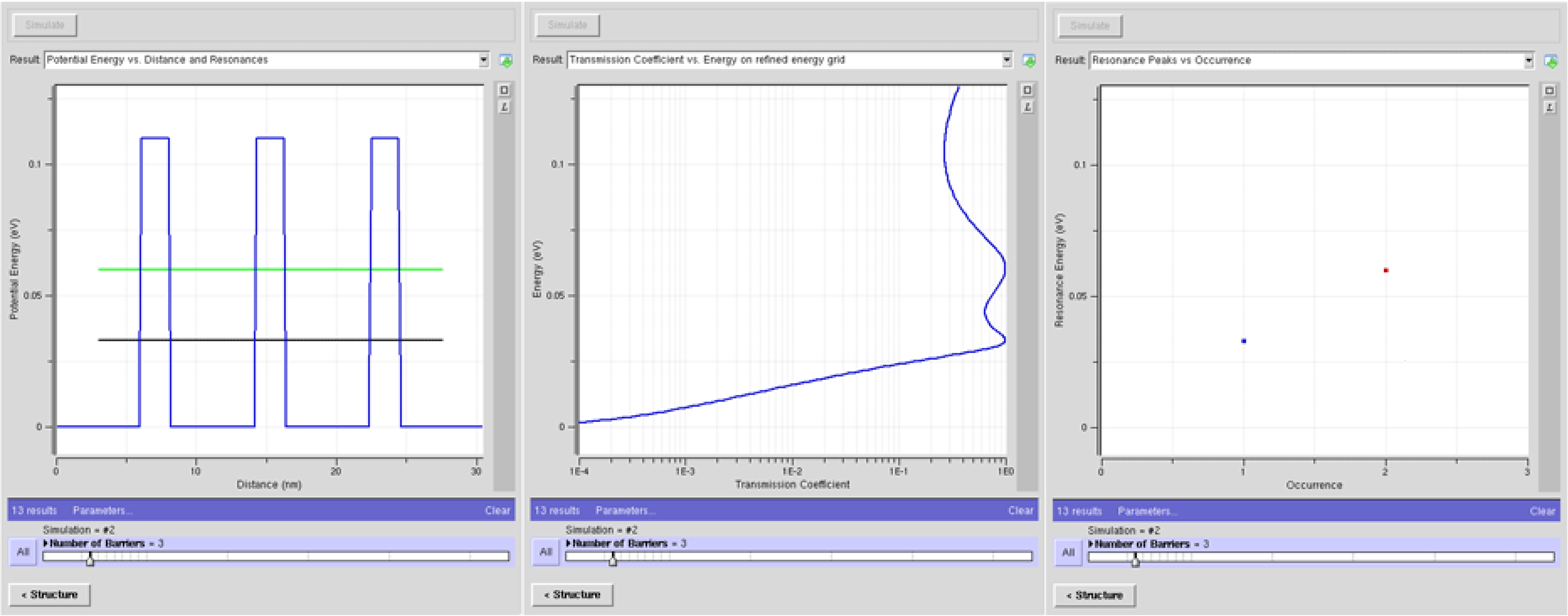
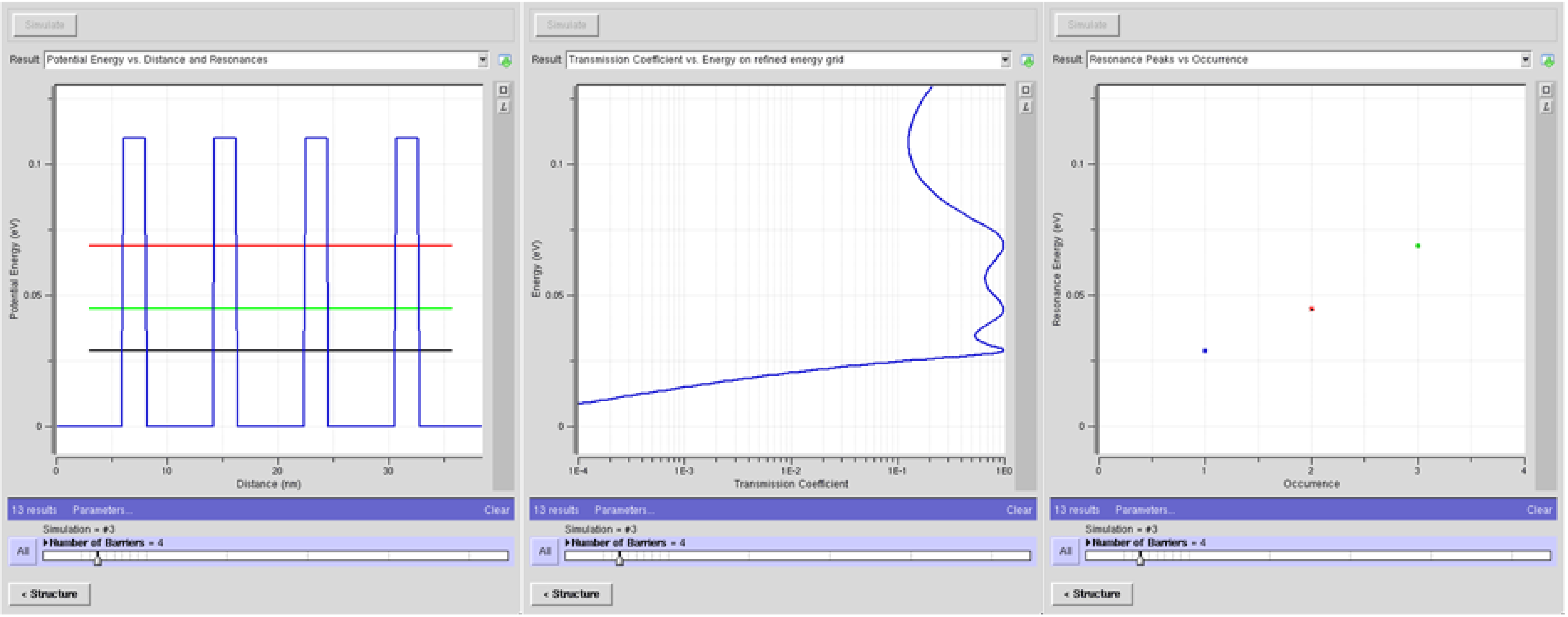
# 2 Wells => 2 Transmission Peaks => 2 States



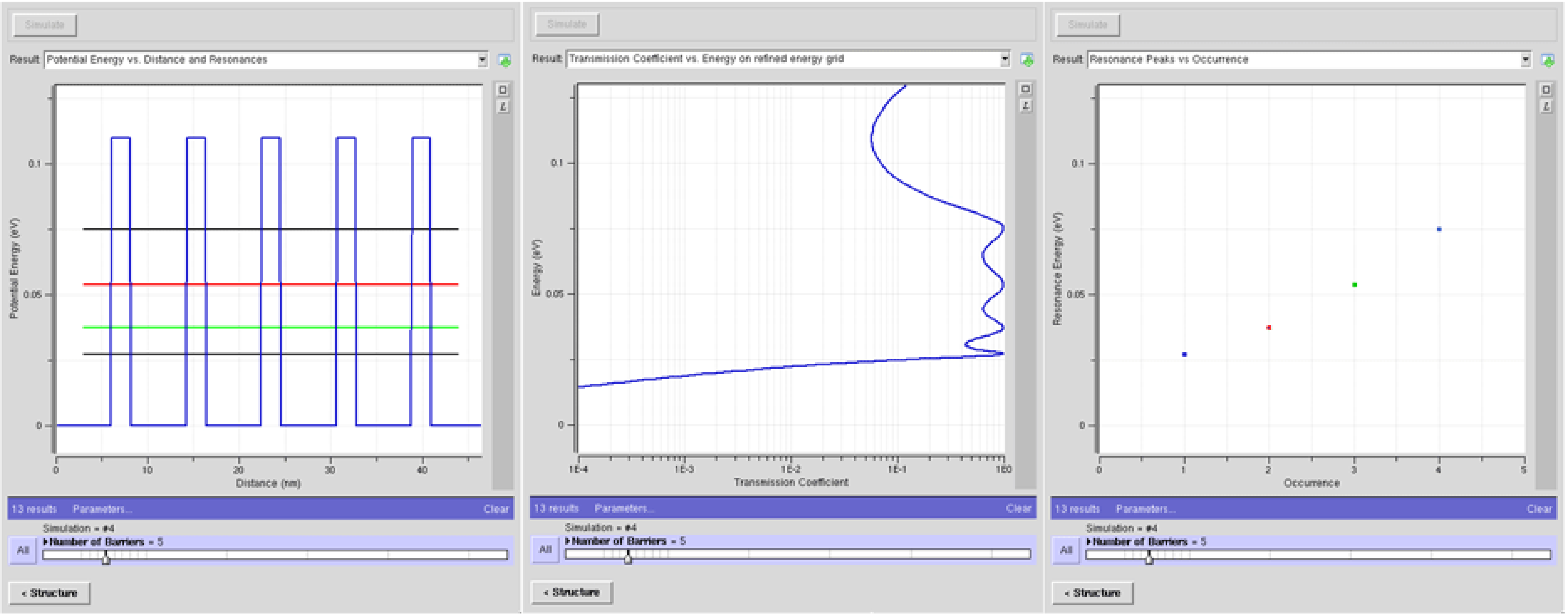

- Bandpass filter formed
- Band transmission not symmetric

# 3 Wells => 3 Transmission Peaks => 3 States



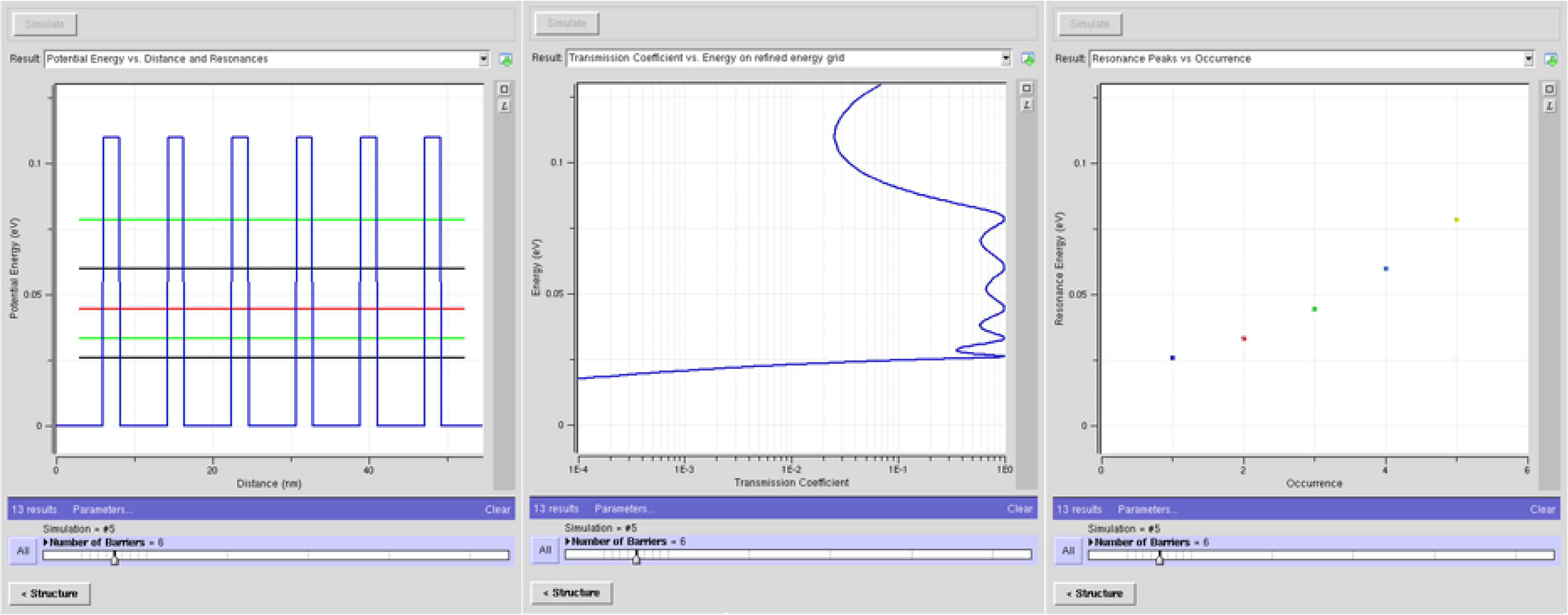

- Bandpass filter formed
- Band transmission not symmetric

# 4 Wells => 4 Transmission Peaks => 4 States



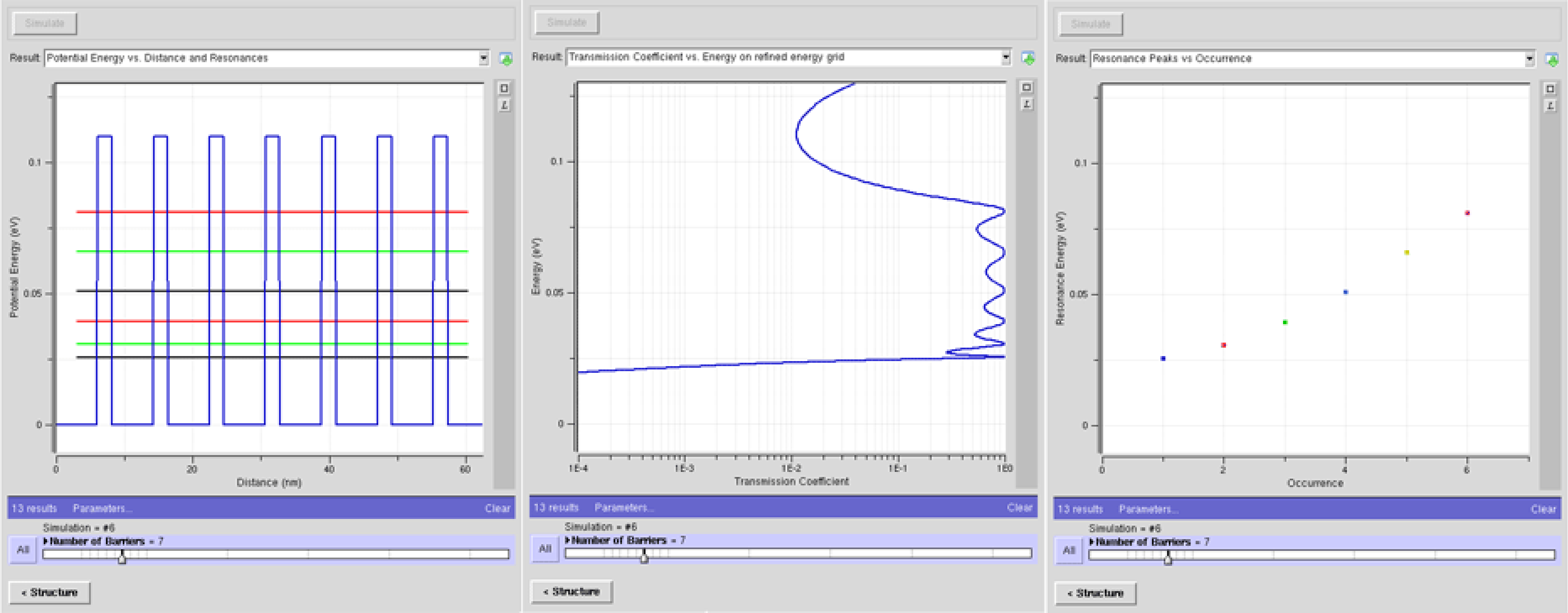

- Bandpass filter formed
- Band transmission not symmetric

# 5 Wells => 5 Transmission Peaks => 5 States



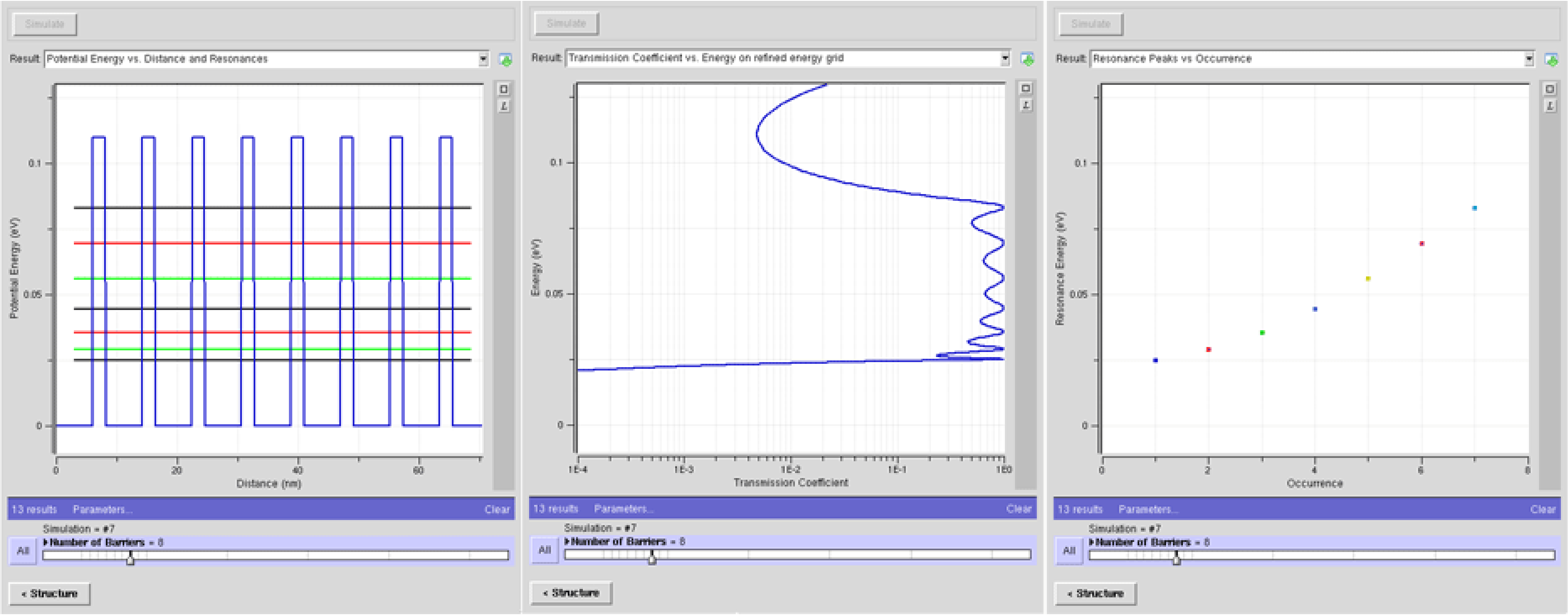

- Bandpass filter formed
- Band transmission not symmetric

# 6 Wells => 6 Transmission Peaks => 6 States



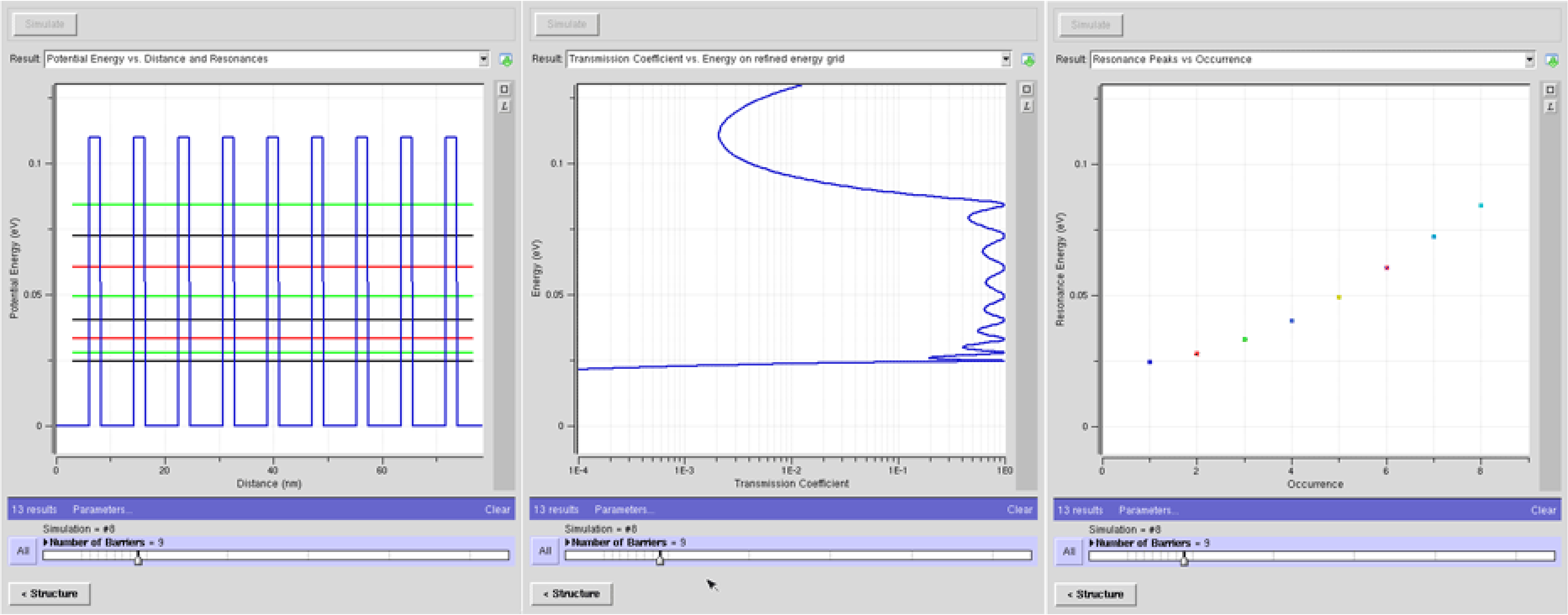

- Bandpass filter formed
- Band transmission not symmetric

# 7 Wells => 7 Transmission Peaks => 7 States



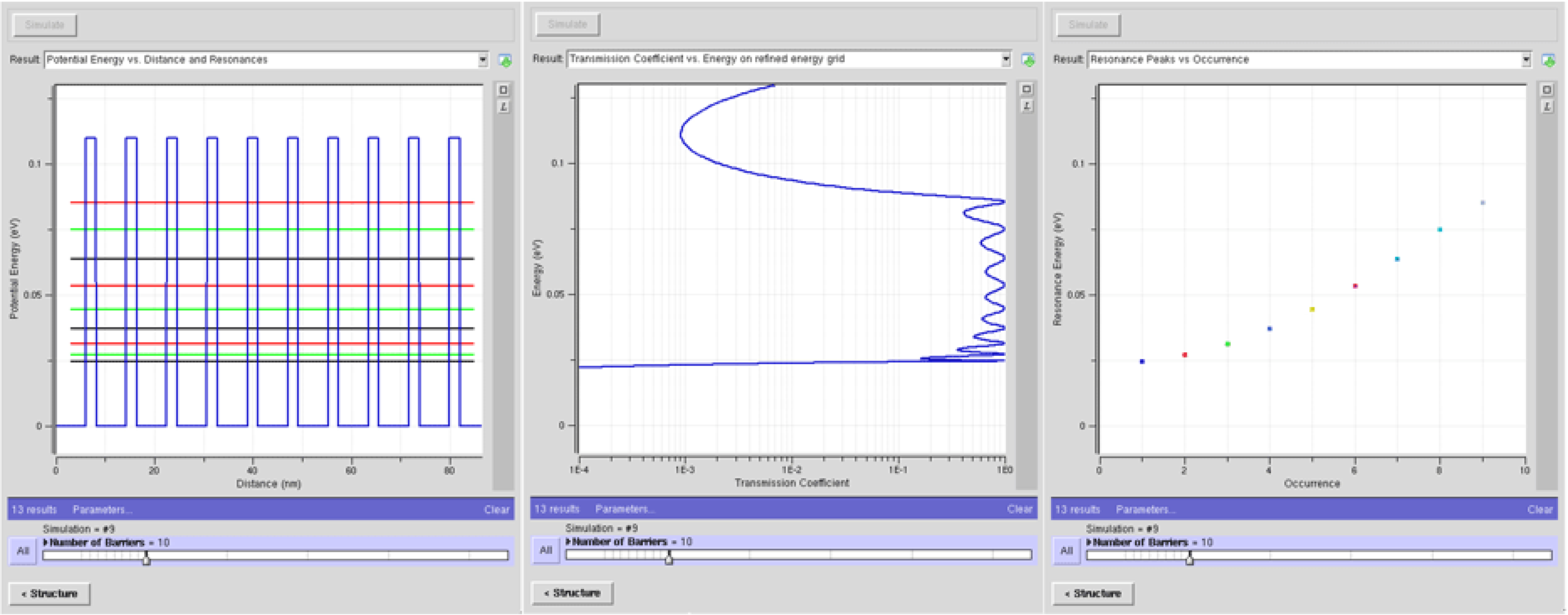

- Bandpass filter formed
- Band transmission not symmetric

# 8 Wells => 8 Transmission Peaks => 8 States



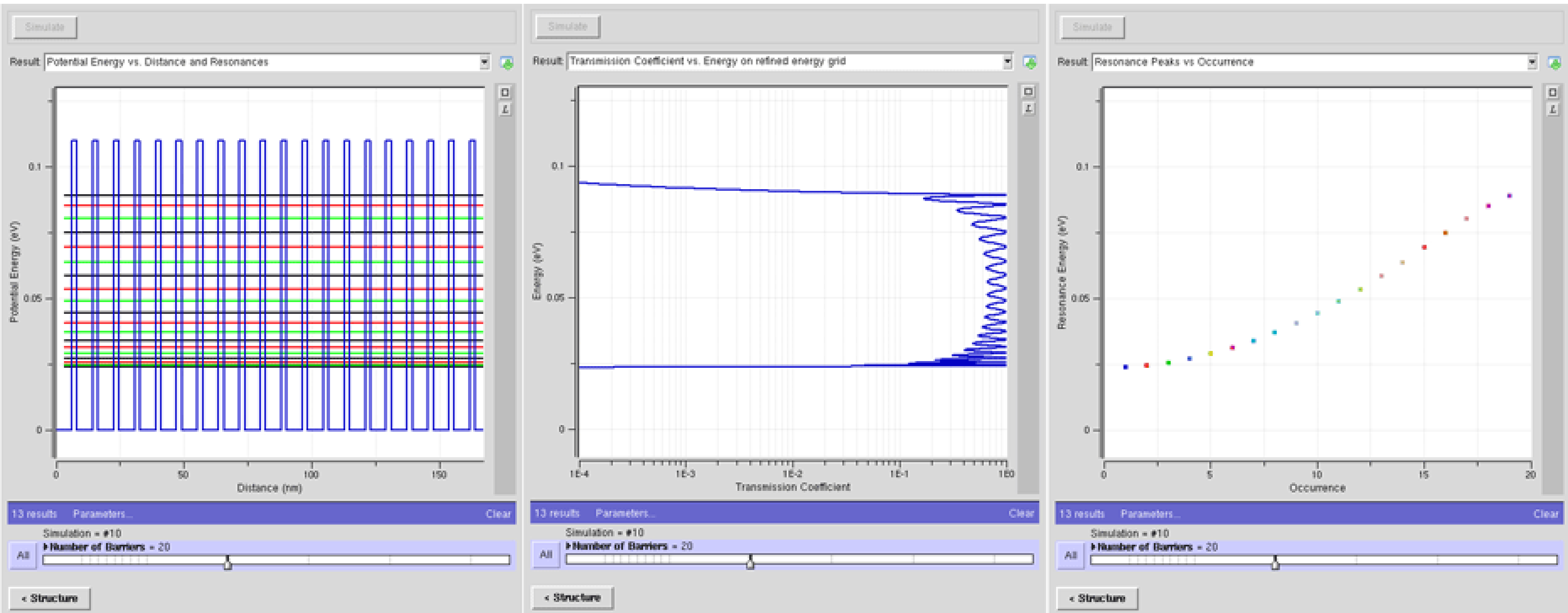

- Bandpass filter formed
- Band transmission not symmetric

# 9 Wells => 9 Transmission Peaks => 9 States



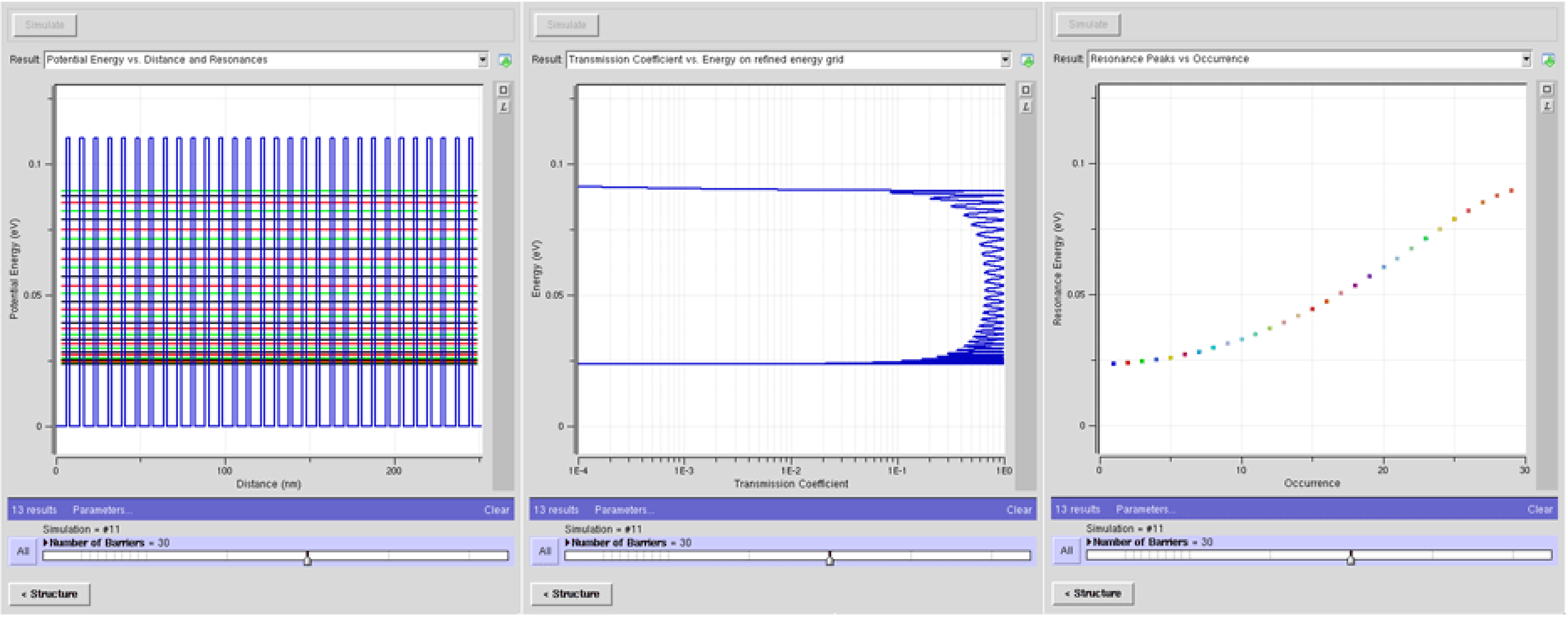

- Bandpass filter formed
- Band transmission not symmetric

# 19 Wells => 19 Transmission Peaks => 19 States



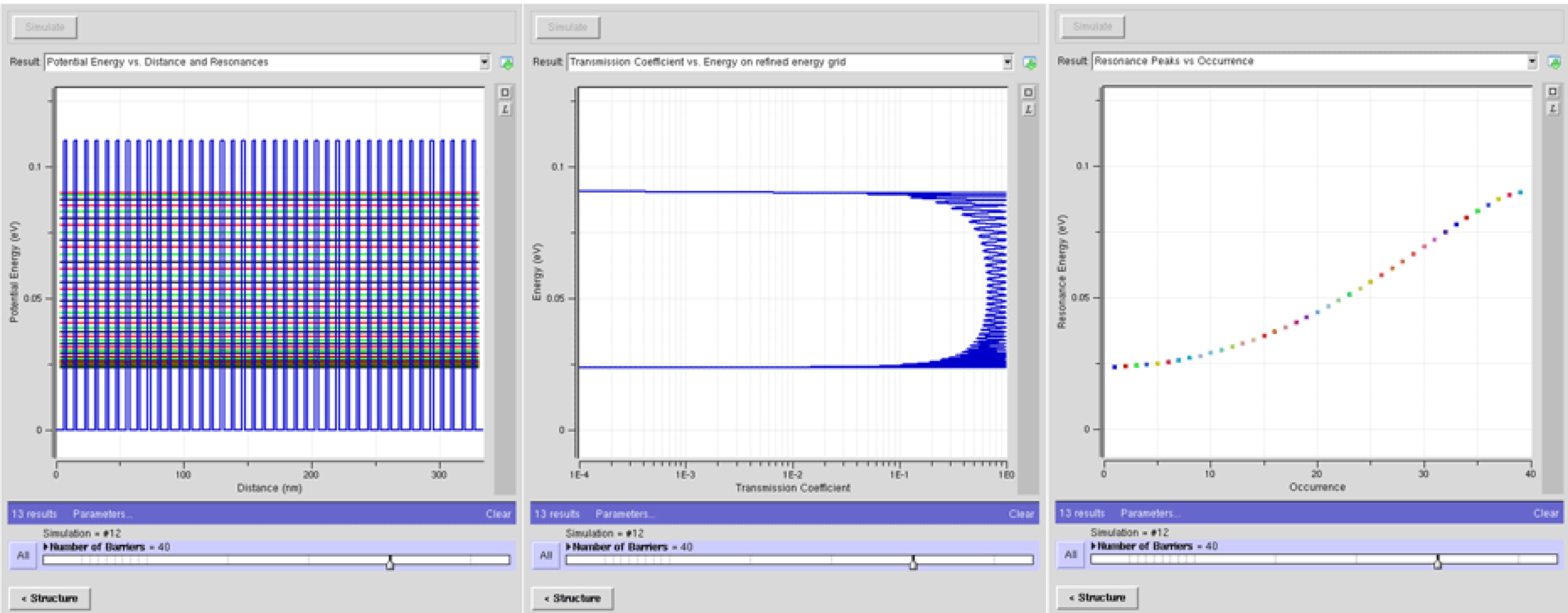

- Bandpass filter formed
- Band transmission not symmetric

# 29 Wells => 29 Transmission Peaks => 29 States



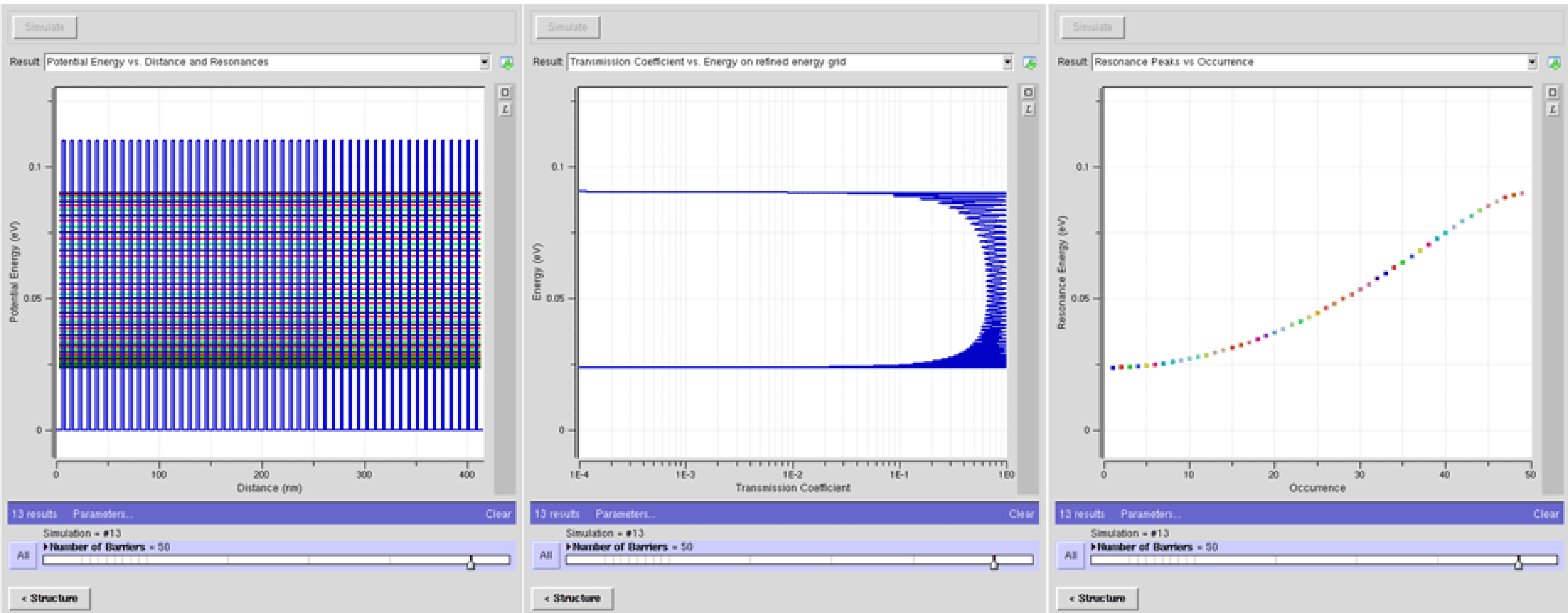

- Bandpass filter formed
- Band transmission not symmetric

# 39 Wells => 39 Transmission Peaks => 39 States



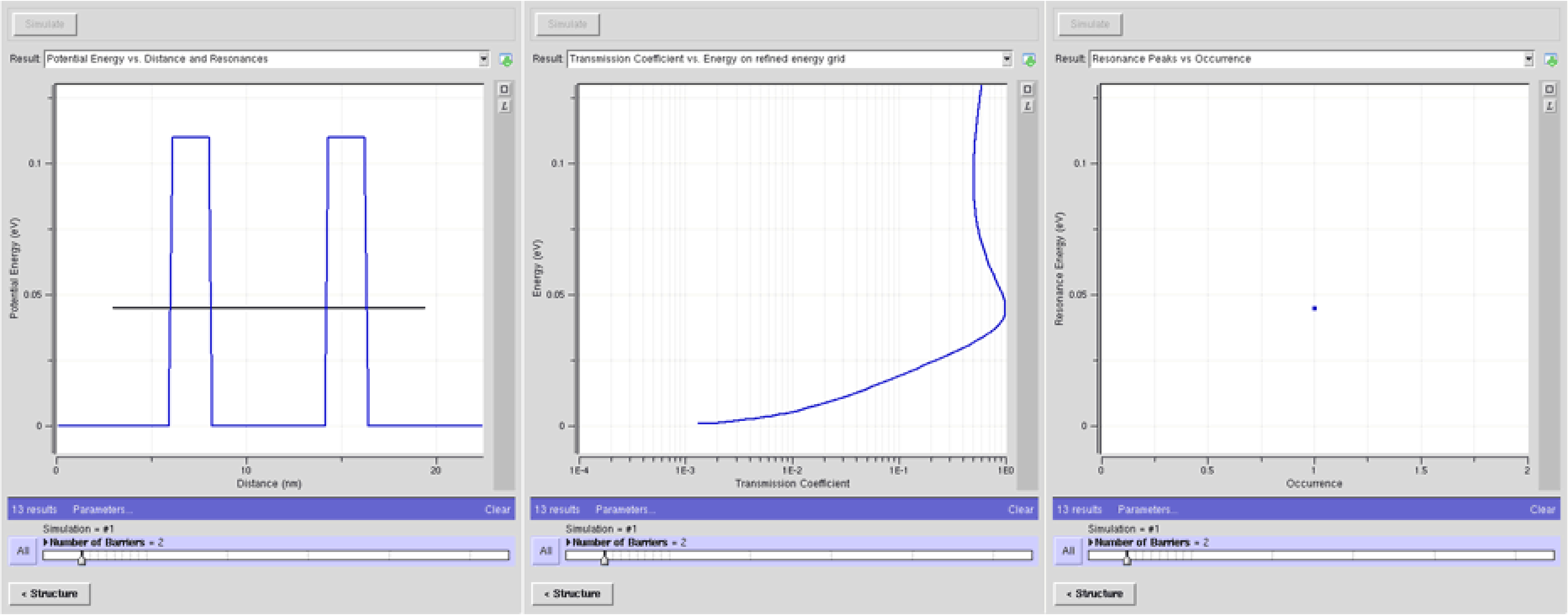

- Bandpass filter formed
- Band transmission not symmetric

# 49 Wells => 49 Transmission Peaks => 49 States




- Bandpass filter formed
- Band transmission not symmetric
- Cosine-like band formed
- Band is not symmetric

# N Wells => N Transmission Peaks => N States

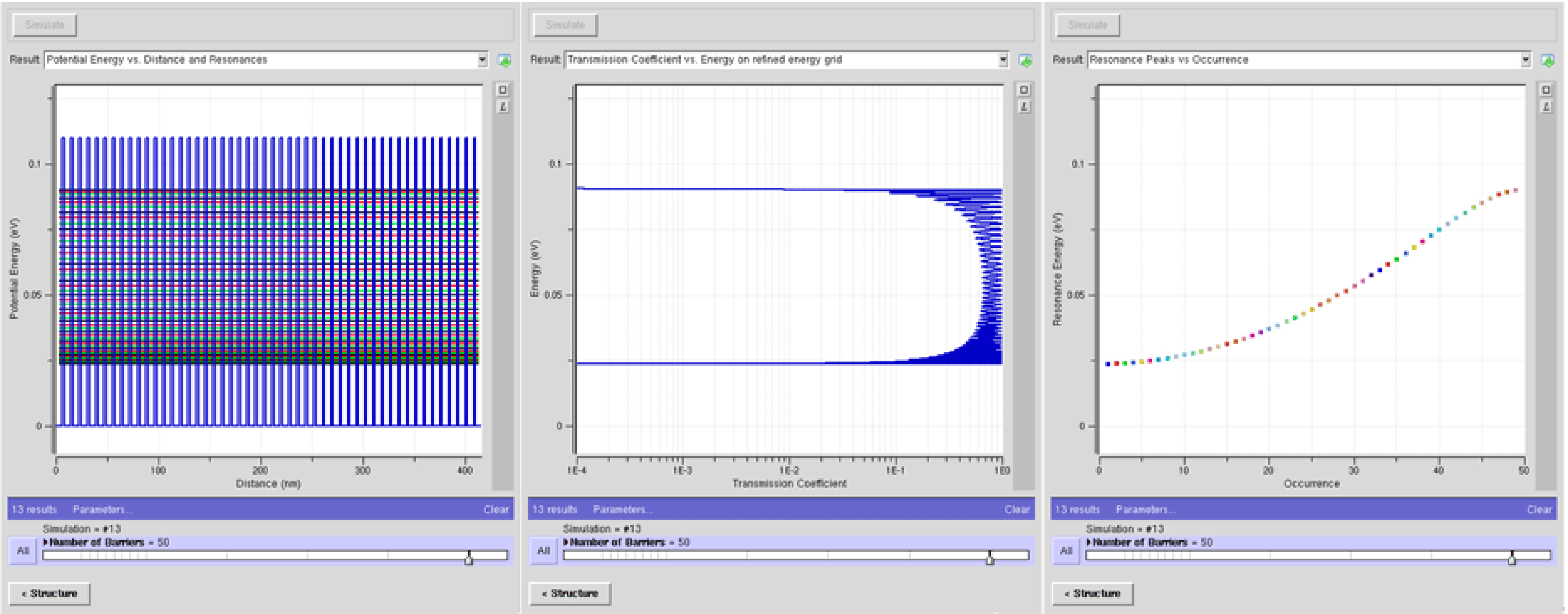



- Bandpass filter formed
- Band transmission not symmetric
- Cosine-like band formed
- Band is not symmetric

# N Wells => N States => 1 Band

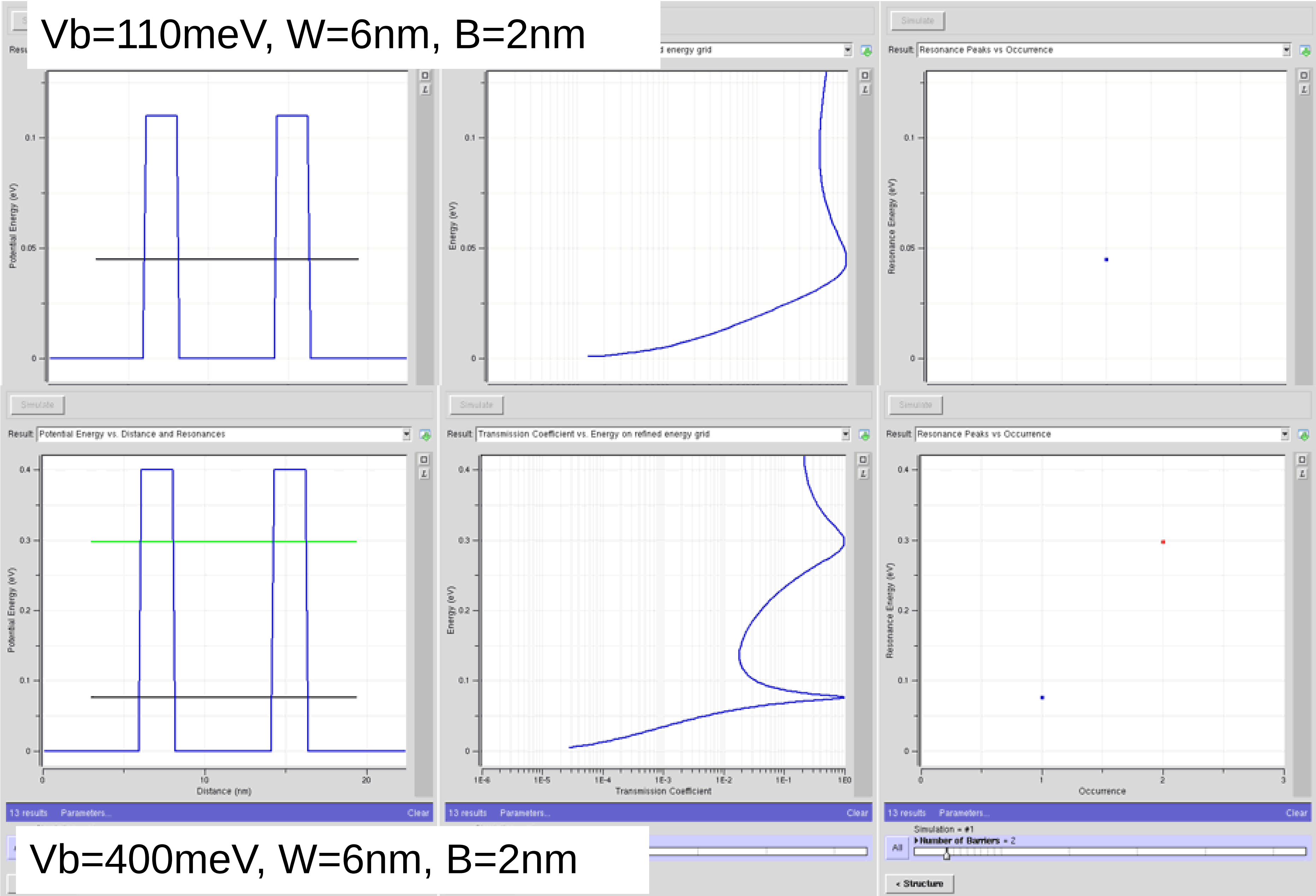
- Vb=110meV, W=6nm, B=2nm => ground state in each well

=> what if there were excited states in each well => Vb=400meV



# N Wells => 2N States => 2 Bands

Vb=110meV, W=6nm, B=2nm

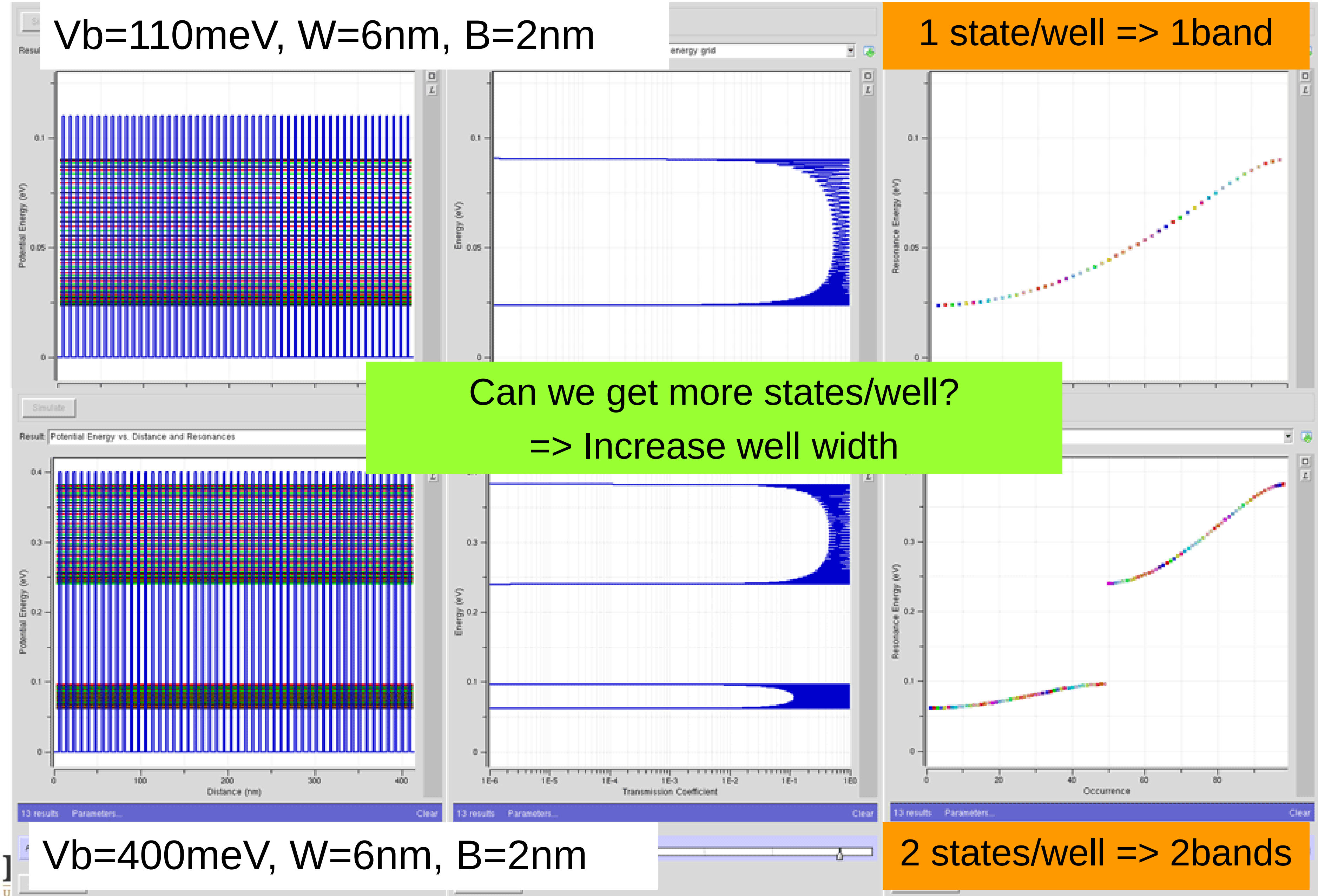



Vb=400meV, W=6nm, B=2nm

# N Wells => 2N States => 2 Bands

Vb=110meV, W=6nm, B=2nm

1 state/well => 1band

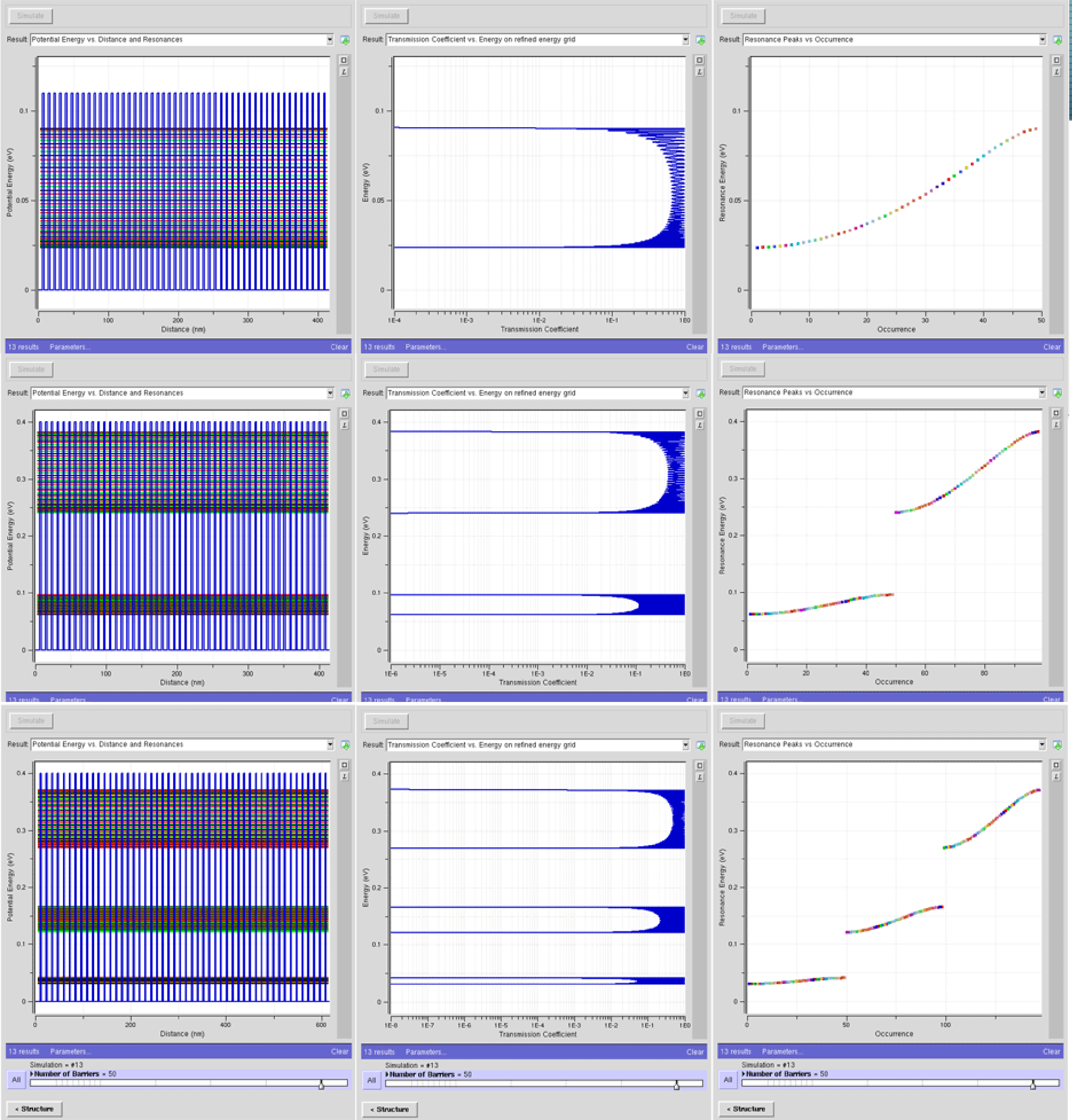



Can we get more states/well?

=> Increase well width

Vb=400meV, W=6nm, B=2nm

2 states/well => 2bands



# X States/Well => X Bands

Vb=110meV,
W=6nm, B=2nm

**1 state/well => 1 band**

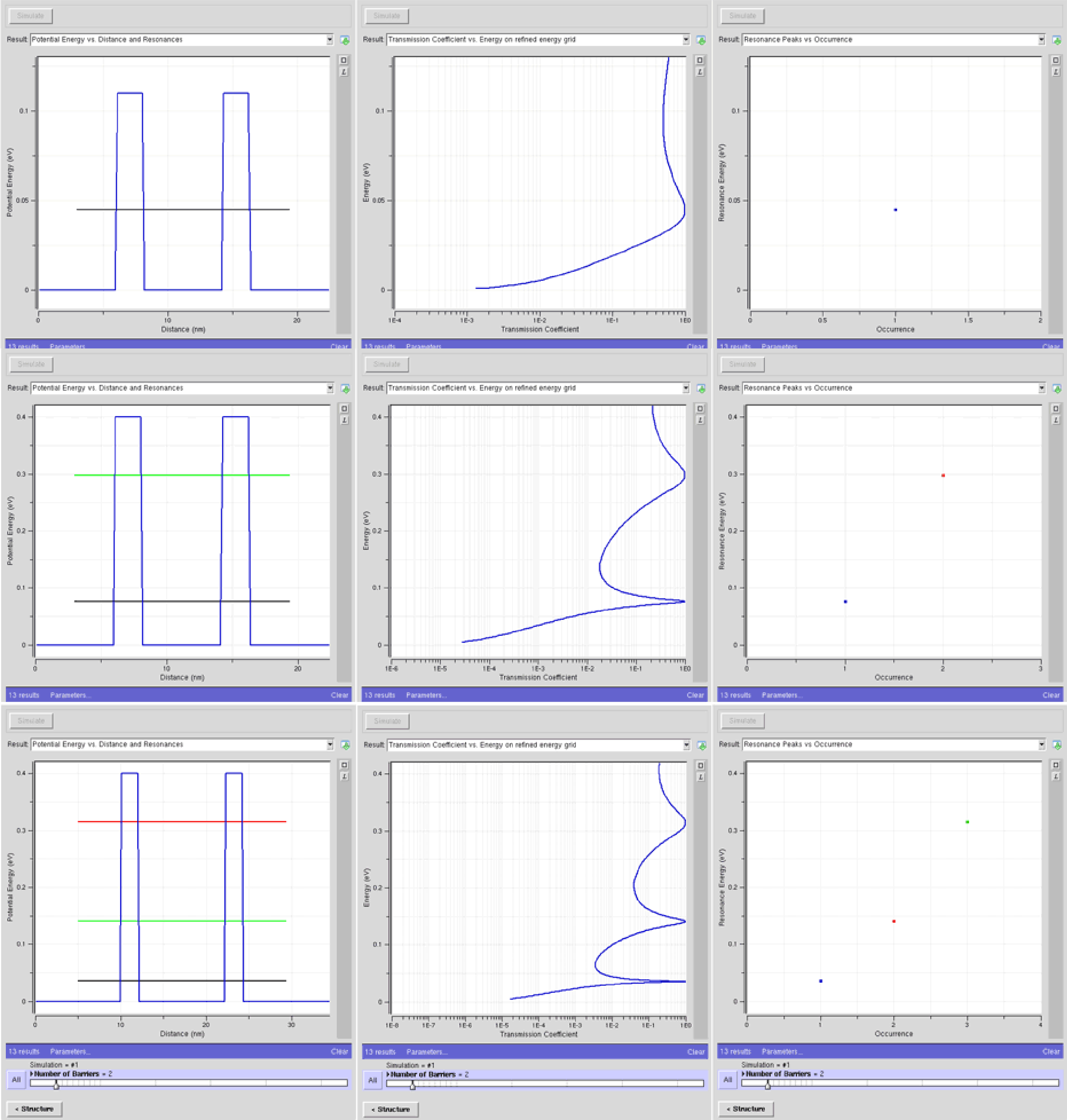
Vb=400meV
W=6nm, B=2nm

**2 states/well => 2 bands**

Vb=400meV
W=10nm, B=2nm

**3 states/well => 3 bands**

# X States/Well => X Bands




Vb=110meV,
W=6nm, B=2nm

**1 state/well => 1 band**

Vb=400meV
W=6nm, B=2nm

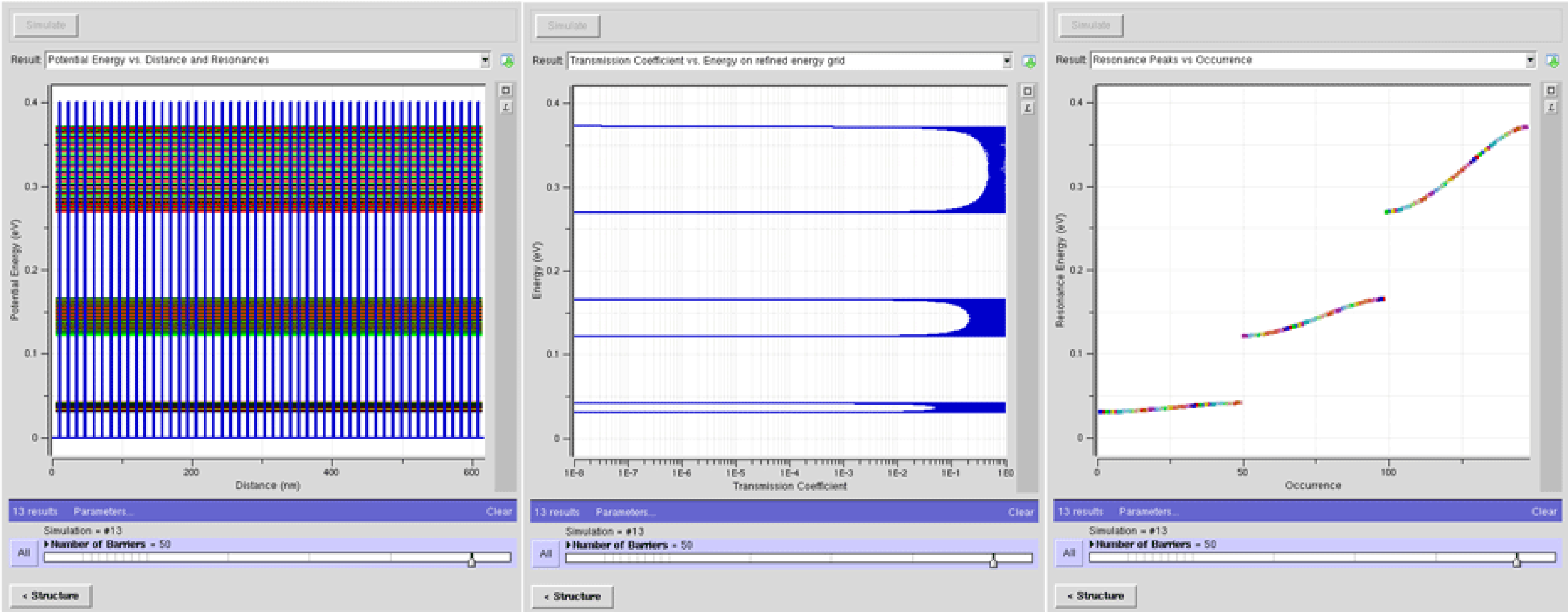
**2 states/well => 2 bands**

Vb=400meV
W=10nm, B=2nm

**3 states/well => 3 bands**

# Formation of energy bands

- Each quasi-bond state will give rise to a resonance in a well. (No. of barriers -1)
- Degeneracy is lifted because of interaction between these states.
- Cosine-like bands are formed as the number of wells/barriers is increased
- Each state per well forms a band
- Lower bands have smaller slope = > heavier mass



# Presentation Outline

- Analytical solutions of Toy Problems
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers

**Reference:**

- piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt