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COMPARATIVE ANALYSIS OF THE TRANSMISSION COEFFICIENTS OF THE 1D RECTANGULAR POTENTIAL BARRIER FOR Ge, Si, GaAs & $Al_{0.37}Ga_{0.63}As$

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ABSTRACT

Python programming is used in the comparative analysis of the transmission coefficients, T, as function of barrier width, "a", barrier height "V_0", and particle energy "E". These variables are chosen in pairs of various combinations, while keeping one of the variables a constant. Four semiconductor materials types [Germanium (Ge), Silicon (Si), Gallium Arsenide (GaAs) and Aluminum Gallium Arsenide ($Al_{0.37}Ga_{0.63}As$)] are chosen and the idealized 1D rectangular single-barrier potential is used as the model. Results show that increasing the particle energy enhances tunneling probability, leading to peaks of 0.79, 0.55, 0.46 and 0.36 at energies 0.50eV for Ge, 0.88eV for Si, 1.19eV for GaAs and 1.69eV for $Al_{0.37}Ga_{0.63}As$ respectively which may indicate resonance. Moreover, irrespective of the choice of (E, V_o) for each material, the transmission coefficient typically decreases exponentially with the increase in the barrier width. This study further reveals that intrinsic semiconductor materials (Ge, Si) support higher tunneling, whereas semiconductor heterostructures (GaAs, $Al_{0.37}Ga_{0.63}As$) suppress transmission. There is a hierarchy of tunneling efficiency across the materials i.e. $T_{Ge} > T_{Si} > T_{GaAs} > T_{Al0.37Ga0.63As}$, which may serve as a pointer in the design of devices such as resonant tunneling diodes, quantum cascade lasers, and tunneling transistors.

Keywords: Barrier Potential, Tunneling, Transmission Coefficient

INTRODUCTION

Quantum mechanical tunneling plays an important role in the operation of many nanoscale semiconductor devices, where electron transport is strongly influenced by material properties and barrier geometry. It is a non-classical phenomenon in which particle(s) can tunnel through a potential barrier, $V(x)$, which is otherwise, classically impossible for particles with energies, E, less than the barrier height, V_o; the incident particle's wavefunction, ψ, decays exponentially inside the barrier but re-emerges on the other side (Griffiths & Schroeter, 2018).

Analytical and numerical studies of one-dimensional quantum systems continue to provide fundamental insight into tunneling behavior and resonance-like transmission features, (Tanimu & Bagudu, 2020; Eyube, *et al*, 2020). This effect is responsible for several important phenomena (physical processes and technologies), such as alpha decay in nuclear physics and the operation of tunnel diodes, resonant tunneling diodes (RTDs), quantum cascade lasers, and high-electron-mobility transistors in electronics (Mukherjee *et al*., 2011; Yadav *et al*., 2020; Duan *et al*., 2023). The quantum tunneling characteristics of various semiconductors are well-characterized by their transmission coefficients, T, which are sensitive functions of particle energy, barrier geometry and intrinsic material properties such as bandgap as well as the effective mass (David, 2005). This sensitivity is crucial in the engineering of nanoscale devices, making this modeling approach both timely and technically robust.

Quantum tunneling phenomena have been investigated using a range of analytical, semi-analytical and numerical approaches, depending on the complexity of the physical system and the objectives of the study. For idealized one-dimensional potentials, analytical solutions of the time-independent Schrödinger equation are often employed because they provide direct physical insight into the transmission behavior (Griffiths & Schroeter, 2018; Eyube et al, 2020).

To extend such analyses, several authors have adopted numerical or matrix-based methods (Tanimu and Bagudo, 2020; Eyube et al., 2020). While these approaches are effective, they are generally tailored to particular systems and may require repeated reformulation when applied to comparative studies involving multiple materials.

In some other related works, proprietary computational platforms such as MATLAB and Mathematica have frequently been employed for tunneling simulations (Ban et al., 2000; Mukherjee et al., 2011). Although these methods are well established and computationally powerful, their reliance on licensed software can limit accessibility and reproducibility, especially for broad parametric studies.

Other studies have utilized transfer-matrix methods, discrete numerical solvers or finite-difference schemes to investigate tunneling in layered or device-specific systems (Supriadi et al., 2019; Duan et al., 2023). These techniques are particularly useful for detailed device modelling but may introduce additional computational complexity when the primary aim is to compare material-dependent trends under uniform modelling conditions.

Despite these advances, most existing studies focus on individual materials or specific heterostructure configurations. Direct comparisons across different semiconductor types are often complicated by variations in model assumptions, barrier geometries or numerical methods. As a result, the relative tunneling efficiencies of commonly used semiconductor materials types under identical physical conditions are not always clearly established.

In this work, Python is employed in the analysis of the transmission coefficients of Ge, Si, GaAs, and $Al_{0.37}Ga_{0.63}As$ within a single, unified computational framework, enabling direct comparison of their tunneling behavior under matched barrier geometries and energy ranges. Python-based

numerical modeling is employed to systematically explore how variations in barrier width, barrier height and particle energy influence transmission. This approach provides transparent visualization of tunneling trends and assumes the isolation of material-dependent effects, as well as preserves the analytical formulation while enabling efficient numerical evaluation over wide ranges of barrier width, effective barrier height, and particle energy. The use of open-source libraries such as NumPy and Matplotlib supports reproducibility and clear visualization of results without introducing hidden solver assumptions.

Moreover, consistent with recent studies that have applied Python-based tools to time-independent quantum mechanical problems (Shahinyan et al., 2024), the present methodology emphasizes clarity and accessibility rather than computational complexity. Given the idealized rectangular barrier model adopted, this approach is appropriate for examining comparative tunneling trends across different types of semiconductor materials while maintaining due caution regarding physical realism. Furthermore, by linking fundamental tunneling probabilities to material choice, this study also aims to bridge simplified quantum models and practical semiconductor device considerations as had been attempted by others (Manga *et al*., 2025).

MATERIALS AND METHODS

Theoretical Framework/Methodology

The system considered is a 1D rectangular potential barrier of width a and height V_o, as illustrated schematically in Figure 1 below (Phillips, 2013).

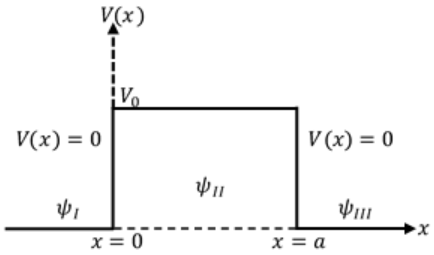

Figure 1: 1D Rectangular Barrier Potential

The potential, $V(x)$ is defined as

$$V(x) = \begin{cases} 0, & -\infty < x < 0 \\ V_0 & 0 < x < a \\ 0, & a < x < +\infty \end{cases} \quad (1)$$

The transmission coefficient, T, for the particle energies, $E < V_o$, is obtained by solving the Time Independent Schrödinger Equation (TISE), as:

$$T = \left[\frac{16E(V_0 - E)}{{V_0}^2}\right] e^{-2\beta a} \quad (2)$$

where, $\beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ (3)

reduced Planck's constant, $\hbar = 1.054 \times 10^{-34} Js$,

the mass of electron, $m = 9.11 \times 10^{-31} kg$.

It is noted that material-specific effective masses are not explicitly included in this idealized model.

Python programming is used to carry out a comparative analysis of the transmission coefficients (eqn 2) of four semiconductors viz Germanium (Ge), Silicon (Si), Gallium Arsenide (GaAs) and Aluminum Gallium Arsenide ($Al_{0.37}Ga_{0.63}As$) using the libraries: NumPy for numerical evaluation and Matplotlib for visualization.

The values of the energy band gaps, E_g, of these semiconductors are used in place of the barrier, V_o, since the energy required to overcome the barrier, V_o, is directly proportional to the semiconductor band gap, E_g, which can be measured with greater accuracy. While this does not represent a detailed heterojunction band offset, it provides a consistent basis for qualitative comparative analysis. The electron energies, E, used are in the range from 0.01eV to a maximum of the barrier height, V_o. Energy step sizes were chosen sufficiently small to ensure smooth transmission curves. Table 1 summarizes the barrier heights used:

Table 1: Barrier Heights of Selected Semiconductors at 300K

S/No	Semiconductor Materials	Barrier Height (V_0) in eV	Particle Energy Range (E) in eV
1.	Germanium (Ge)	0.67	0.01 – 0.67
2.	Silicon (Si)	1.12	0.01 – 1.12
3.	Gallium Arsenide (GaAs)	1.42	0.01 – 1.42
4.	Aluminum Gallium Arsenide ($Al_{0.37}Ga_{0.63}As$)	1.91	0.01 – 1.91

The transmission coefficients, T, of Germanium (Ge), Silicon (Si), Gallium Arsenide (GaAs) and Aluminum Gallium Arsenide ($Al_{0.37}Ga_{0.63}As$) are evaluated as a function of barrier width, "a", barrier height "V_0", and incident particle energy "E" chosen in pairs of various combinations, while keeping one of the variables a constant, i.e $T(a, E)|_{V_0=0.67eV}$, $T(a, V_0)|_{E=0.07eV}$, $T(V_o, E)|_{a=0.1nm}$ and $T(E, V_o)|_{a=0.3nm}$.

RESULTS AND DISCUSSION

Transmission Coefficient of Ge as a Function of Barrier Width and Particle Energy with Constant Barrier Height, $T(a, E)|_{V_o=0.67eV}$

Figure 2, below, shows the python script to obtain $T(a, E)|_{V_o=0.67eV}$ for germanium, Ge, $(V_o = 0.67eV)$ at different particle energies, corresponding for energy values of $E = 0.02eV, 0.04eV, 0.06eV$ and $0.08eV$.

```python
import numpy as np
import matplotlib.pyplot as plt

hbar = 1.054e-34 # Reduced Planck's constant (J·s)
m = 9.11e-31    # Electron mass (kg)
a = np.linspace(0.1, 0.3, 200) * 1e-9  # Barrier width (m)

plt.figure(figsize=(8, 6))

E_values = [0.02, 0.04, 0.06, 0.08] #Energy Values (eV)
v = 0.67*1.602e-19   #Barrier Height for Ge (J)

colorsA=['red', 'black', 'green', 'brown']

for i, E1 in enumerate(E_values):

    E = E1 * 1.602e-19     #Energy in eV to Joules
    beta = np.sqrt(2 * m * (v - E)) / hbar
    X = np.exp(-2 * beta * a)
    T = ((16 * E * (v - E))/v**2) * X  #Transmission Coefficient

    plt.plot(a, T, linewidth=2, label=f'$E={E1}eV$, $V_0=0.67eV$', color=col

plt.xlabel('Barrier Width (a) in meter')
plt.ylabel('Transmission Coefficient (T)')
plt.legend()
#plt.title("Graph of T(a) for Ge with four different values of Energy(E)")
plt.grid(alpha=0.3)

plt.show()
```

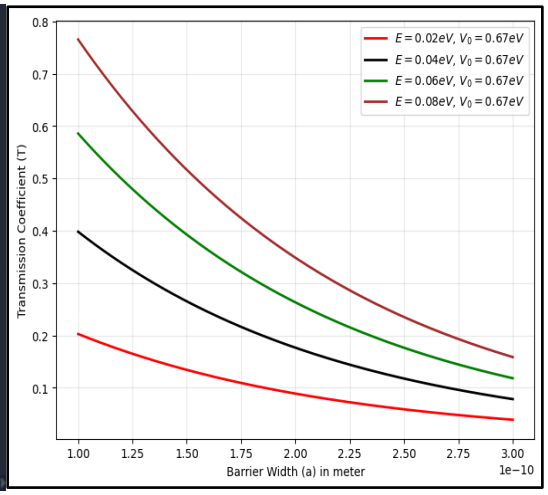

Figure 2: T(a) of Germanium, Ge (Vo = 0.67eV), for four Different Particle Energies, E

It is observed that, for a fixed barrier height, the transmission coefficient, T , displays a slow and uniform exponential decrease as the barrier width, "a", increases; moreover, the rate of the decrease of the transmission coefficient increases with the particle energy, E. Furthermore, higher particle energies consistently result in larger tunneling probabilities which reflects the role of the incident energy in enhancing tunneling. This behavior arises from the exponential decay of the electron wavefunction inside the barrier with thicker barriers leading to stronger attenuation. Higher particle energies reduce the decay constant, allowing greater penetration and hence higher transmission probabilities.

Transmission Coefficients of Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$ as a Function of Barrier Width and Barrier Height when Particle Energy, E is Constant, $T(a, V_o)|_{E=0.07eV}$

The transmission coefficients of Germanium (Ge), Silicon (Si), Gallium Arsenide (GaAs) and Aluminum Gallium Arsenide ($Al_{0.37}Ga_{0.63}As$) plotted against the barrier widths, "a" in order to investigate the effect of barrier height when particle energy is kept constant at $E = 0.07eV$ is shown in Figure 3.

```python
import numpy as np
import matplotlib.pyplot as plt

hbar = 1.054e-34 # Reduced Planck's constant (J·s)
m = 9.11e-31    # Electron mass (kg)
a = np.linspace(0.1e-9, 0.3e-9, 200)  # Barrier width (m)

plt.figure(figsize=(8, 6))
E0 = 0.07*1.602e-19 #Energy Value (J)

#Barrier Heights (eV) for Ge, Si, GaAs and Al_0.37Ga_0.63As repectively
v0_values = [0.67, 1.12, 1.43, 1.91]

colorsB=['orange', 'grey', 'teal', 'magenta']
for i, v1 in enumerate(v0_values):

    v0 = v1 * 1.602e-19   #Barrier heights in eV to J
    beta = np.sqrt(2 * m * (v0 - E0)) / hbar
    X = np.exp(-2 * beta * a)
    T = (((16 * E0 * (v0 - E0))/v0**2) * X)  #Transmission Coefficient

    plt.plot(a, T, linewidth=2, label=f'$V_0={v1}eV$, E = 0.07eV',
             color=colorsB[i])

plt.xlabel('Barrier Width (a) in meter')
plt.ylabel('Transmission Coefficient (T)')
#plt.title("Graph of T(a) for different values of Barrier Height(V0)")
plt.legend()
plt.grid(alpha=0.3)
plt.show()
```

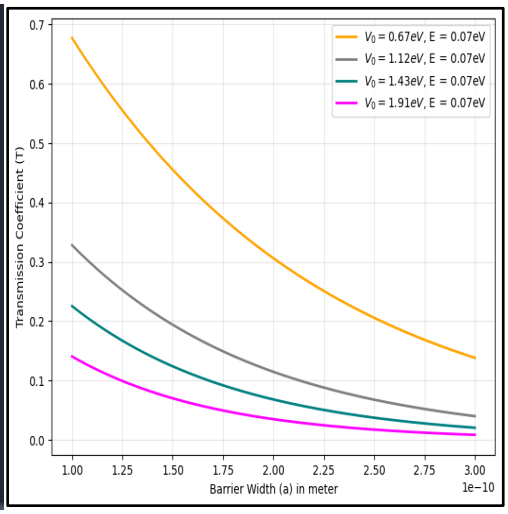

Figure 3: T(a) of Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$ at Constant Particle Energy, E

The Figure shows that the transmission coefficients, $T(a, V_o)|_{E=0.07eV}$, also typically decreases exponentially with increasing barrier width. This decrease, which is more pronounced for Ge, is visible across all four materials, but the relative spread highlights how material choice fundamentally governs tunneling. Moreover, the rate of the decrease in the transmission coefficients differ significantly between materials. For example, at widths below $0.3nm$, Ge exhibits much higher tunneling probabilities than $Al_{0.37}Ga_{0.63}As$, due to its smaller bandgap. The material hierarchy, in terms of the transmission coefficient at the same particle energy becomes clear i.e. $T_{Ge} > T_{Si} > T_{GaAs} > T_{Al0.37Ga0.63As}$; this implies that intrinsic semiconductors, with lower bandgaps (Ge, Si), support higher tunneling, whereas semiconductor heterostructure, with larger bandgap ($Al_{0.37}Ga_{0.63}As$), suppress the transmission coefficient. These trends are consistent with established tunneling theory and highlights the strong influence of intrinsic material properties in agreement with Yadav *et al*., (2020). This result suggests that tunneling may be material-dependent.

Comparative Analysis of $T(a, E)|_{V_o=0.67eV}$ and $T(a, V_o)|_{E=0.07eV}$

The combined graphs of $T(a, E)|_{V_o=0.67eV}$ and $T(a, V_o)|_{E=0.07eV}$ is displayed in Figure 4 below

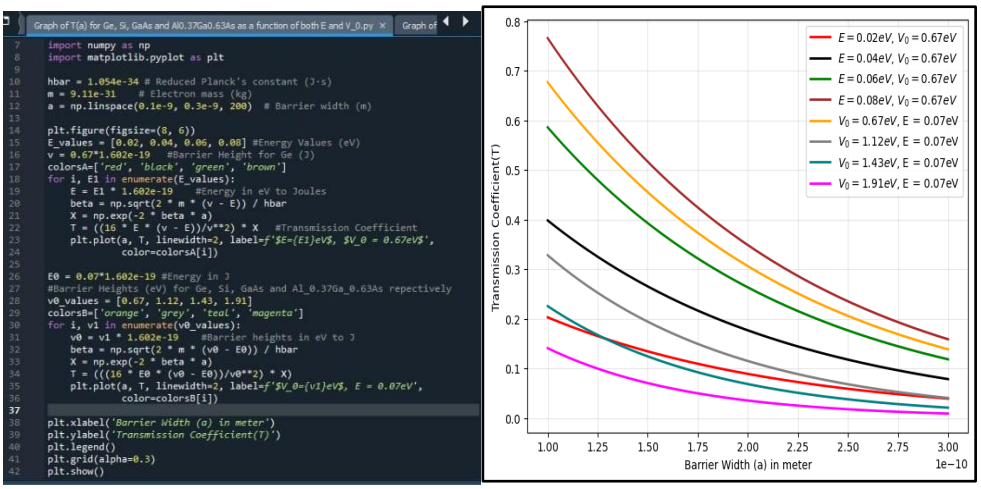

Figure 4: Transmission Coefficients, T(a) Curves for Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$ as a Function of Both E and V_0

This Figure reveal that, irrespective of the pair (E, V_o), the transmission coefficient, T, decreases exponentially with the increase in the barrier width, a. However, for (E, V_o)-pair and $a \leq 0.3nm$, the effect of the particle energy, E, on the transmission coefficient is more predominant than the effect of the barrier height, V_o, for relatively small E. Furthermore, at higher energies, (E, V_o)-pair demonstrates no preferential effect on the transmission coefficient. This dual analysis further demonstrate that particle energy promotes tunneling while higher barriers hinder it. Material-specific differences emerge clearly, with Ge maintaining the highest tunneling probability and $Al_{0.37}Ga_{0.67}As$ the lowest.

Transmission Coefficient as a Function of Barrier Height and Particle Energy when Barrier Width is Constant, $T(V_o, E)|_{a=0.1nm}$

Taking a range of barrier heights $0.67eV \leq V_o \leq 1.91eV$ i.e the range of barrier heights of Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$. Figure 5 displays $T(V_o, E)|_{a=0.1nm}$ for particle energies, E = 0.02eV, 0.04eV, 0.06eV and 0.08eV respectively.

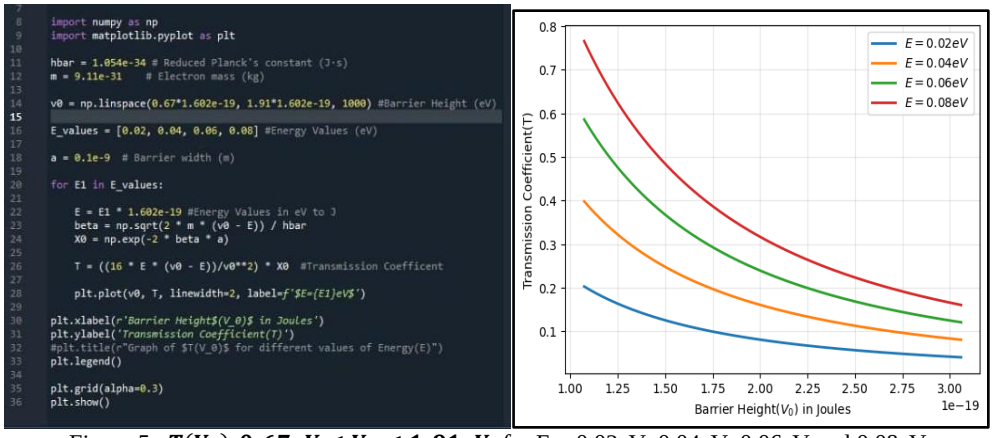

Figure 5: $T(V_o), 0.67eV \leq V_o \leq 1.91eV$, *for* E = 0.02eV, 0.04eV, 0.06eV and 0.08eV

This Figure reveals that the transmission coefficient, $T(V_o, E)|_{a=0.1nm}$, is enhanced with increase in the particle energies,E, similar to the variation with the barrier width, "a". Furthermore, $T(V_o, E)|_{a=0.1nm}$ decreases exponentially with higher barrier heights, V_0. However, this suppression is less at higher particle energies, E. Therefore, it may be inferred that the transmission coefficient, $T(V_o, E)|_{a=0.1nm}$, is higher with lower barrier height and higher particle energy across the four materials. This is in agreement with the works done by Supriadi et al., (2019) and Yadav et al., (2020).

Transmission Coefficient of Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$ as a Function of Particle Energy and Barrier Height when Barrier Width is Constant, $T(E, V_o)|_{a=0.3nm}$

Figure 6 is the transmission coefficient of Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$ as a function of particle Energies and barrier heights when barrier width is kept constant at $0.3nm$,

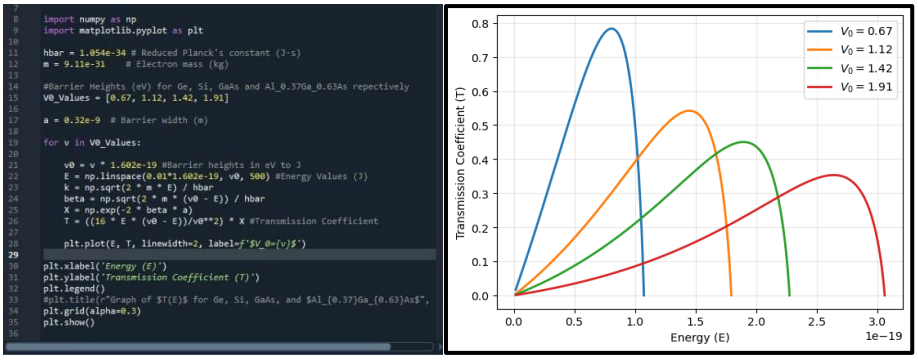

Figure 6: Graph of T(E) for Ge, Si, GaAs and $Al_{0.37}Ga_{0.63}As$

The above Figure shows an initial increase in the transmission coefficient, T as the particle energy, E, increases, which peaks at 0.79, 0.55, 0.46 and 0.36 respectively for particle energies of 0.50eV for Ge, 0.88eV for Si, 1.19eV for GaAs and 1.69eV for $Al_{0.37}Ga_{0.63}As$ respectively. This suggests possible resonant transmission coefficient peaks in line with the work of Mukherjee *et al*. (2011) on $GaAs/AlGaAs$ systems. True resonant tunneling is more rigorously associated with multi-barrier systems (Tanimu & Bagudu, 2020). It is observed that, *Ge* and *Si* exhibit higher amplitudes at lower energies than *GaAs* and $Al_{0.37}Ga_{0.63}As$, suggesting that intrinsic semiconductors support higher tunneling efficiency than semiconductor heterostructures at resonance. These differences further suggest that material choice may directly influences resonance-based devices. This validates the quantum mechanical prediction of resonance tunneling and shows that resonance sharpness diminishes with increasing barrier height.

CONCLUSION

This paper presents a computational analysis of transmission coefficients of *Ge*, *Si*, *GaAs*, and $Al_{0.37}Ga_{0.63}As$ as functions of the barrier width, *a*, the barrier height, V_0, and the particle energy, *E*, chosen in pairs of various combinations, $T(a,E)|_{V_0=0.67eV}$, $T(a,V_0)|_{E=0.07eV}$, $T(V_o,E)|_{a=0.1nm}$ and $T(E,V_o)|_{a=0.3nm}$ with the use of Python. This analysis reveals that intrinsic semiconductors set a fundamental hierarchy of tunneling probabilities. At small widths and low energies, the transmission coefficients, T, *of Ge* is consistently highest, while $Al_{0.37}Ga_{0.63}As$ consistently suppresses it. This provides a predictive framework for selecting semiconductor barriers depending on whether tunneling is desired (RTDs, tunneling FETs) or suppressed (isolation barriers in heterostructures). These findings align with theoretical expectations and highlight the use of Python in bridging analytical models with computational visualization. Beyond educational value, the study highlights the value of simplified computational models in clarifying material trends relevant to semiconductor device engineering.

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