

Development of simulation tools for devices based on magnetic semiconductors

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PhD supervisor: Antonio García Loureiro



Centro Singular de Investigación
en Tecnoloxías da
Información

Contents

- 1 Context: Spintronics
- 2 Hypothesis and Objectives
- 3 Simulation strategy
- 4 Results
- 5 Conclusions



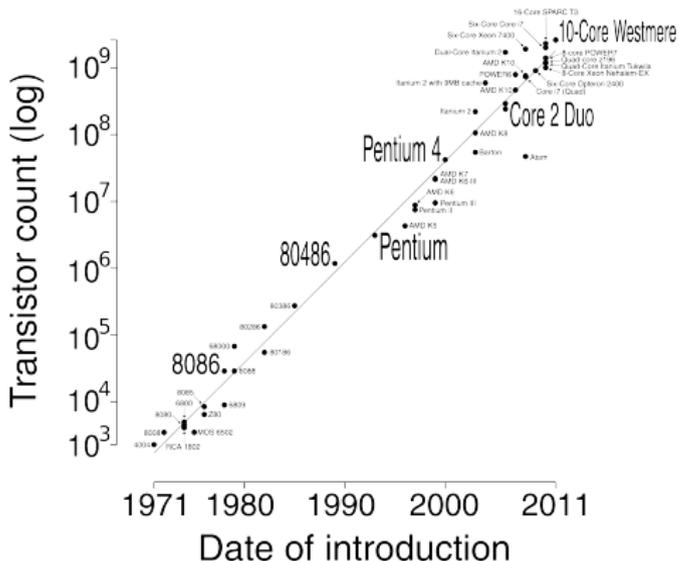
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Integration limit! Moore's Law

Microprocessor Transistor Counts 1971-2011 & Moore's Law



2011:

Westmere-EX (32 nm).

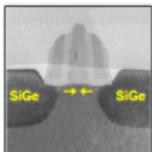
2012:

Ivy Bridge-HE-4 (22 nm).

The complexity for minimum component costs increases at a rate of roughly a factor of two per year.

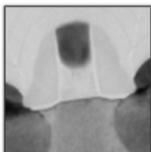
Integration limit! ITRS

2003

90 nm

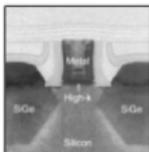
Invented
SiGe
Strained Silicon

2005

65 nm

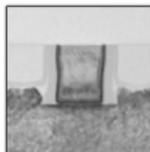
2nd Gen.
SiGe
Strained Silicon

2007

45 nm

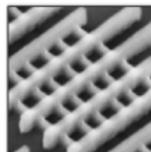
Invented
Gate-Last
High-k
Metal Gate

2009

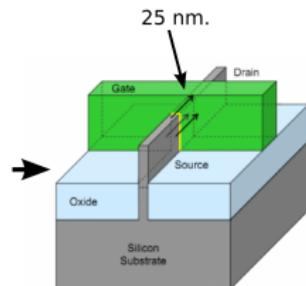
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22 nm

First to
Implement
Tri-Gate



22 nm technological node

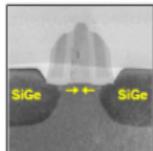
$$25 \text{ nm gate length} \times \frac{1 \text{ silicon cell}}{0,5 \text{ nm}} \times \frac{8 \text{ silicon atoms}}{1 \text{ silicon cell}} \sim 350 \text{ atoms!!}$$

Typical doping: 1 impurity atom per million of silicon.

Then, maybe, no doping in the device!!!

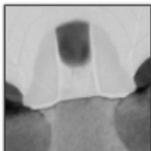
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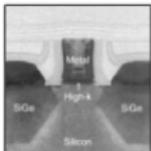
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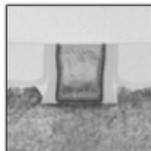
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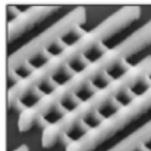
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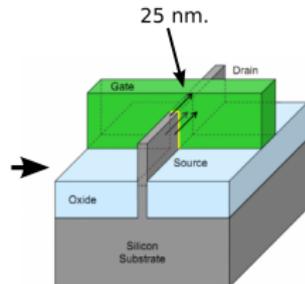
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Integration limit! ITRS

Reduction problems

- ▷ Different device properties under same fabrication conditions.
- ▷ Loss of control on the transistor current.
- ▷ Leakage currents (Tunnel current).
- ▷ More energy density (Heating!).
- ▷ Quantum phenomena.

“Traditional” solutions

- ▷ Increasing doping (Degenerate semiconductors).
- ▷ Exotic geometries (Double gate, Trigate, nanowires...).
- ▷ New materials to avoid leaking (High-K oxides).
- ▷ Reduction of the ON/OFF voltage/current levels.
- ▷ New physical models (Density-gradient, Green, Schrödinger).

Integration limit! ITRS

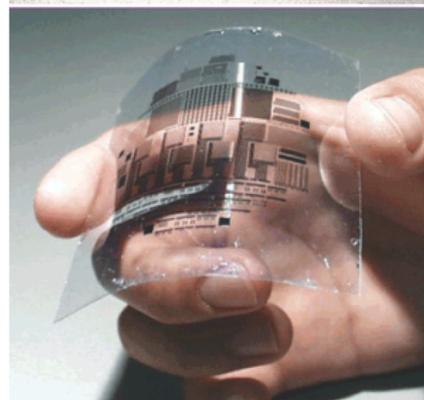
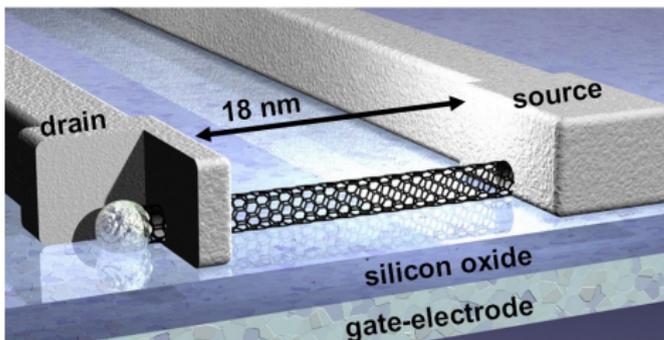
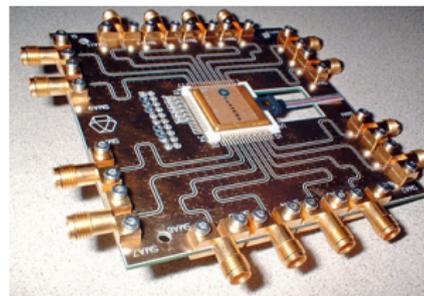
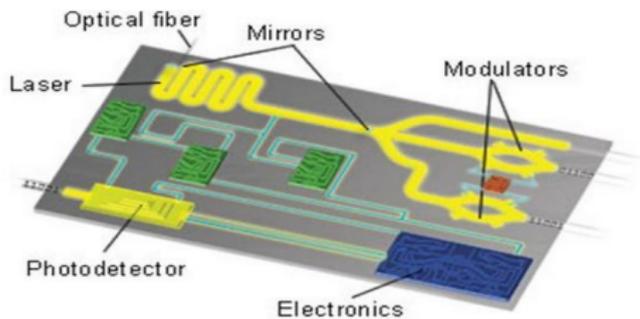
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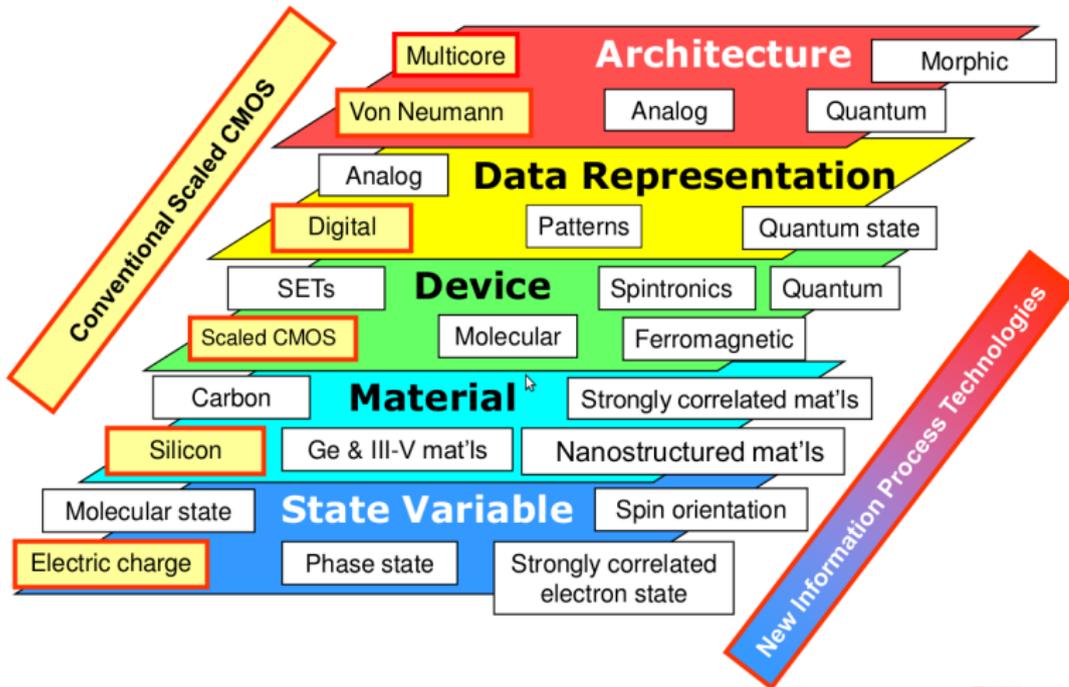
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Alternatives to Electronics



ITRS Alternative: Spintronics?

Emerging Research Devices



International Technology Roadmap for Semiconductors

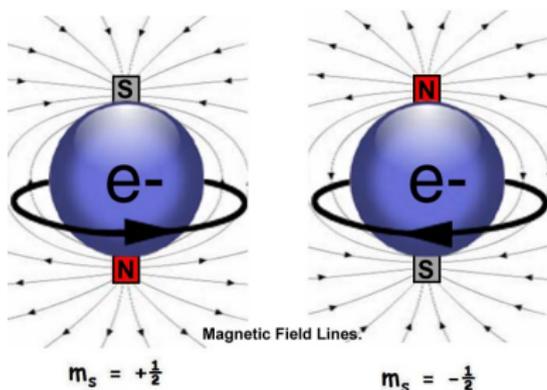


1 ERD WG 4/10/11 Potsdam, Germany - FxP Meeting

Work in Progress -- Not for Publication

What is electron spin?

Spin is an intrinsic form of angular momentum carried by elementary particles.

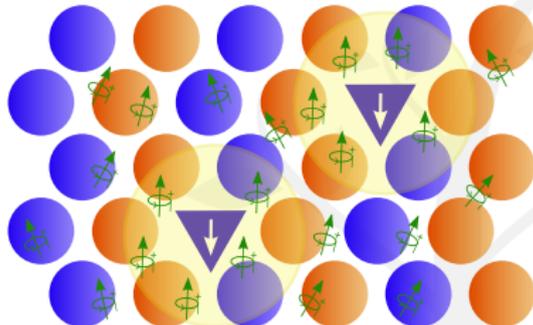


Diluted Magnetic Semiconductors (DMS)

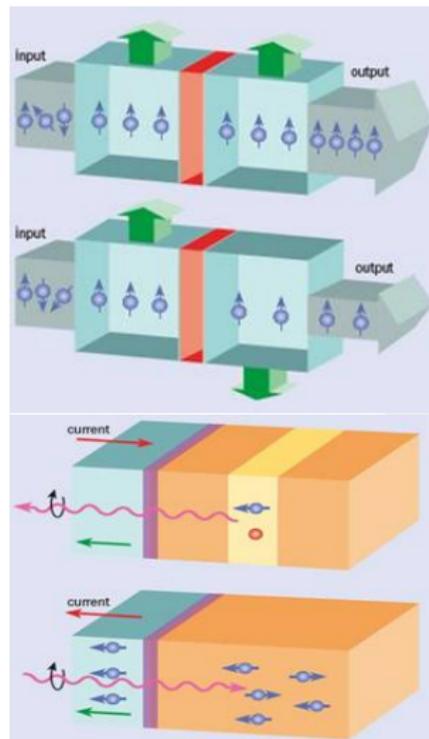
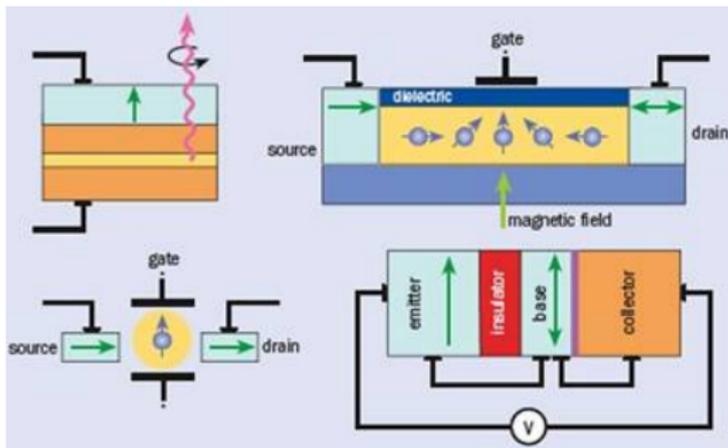
- ▷ Magnetic semiconductors: Integration with electronics.
- ▷ Spin polarization control. Intrinsically and/or externally.
- ▷ Good at $T \sim 0$ K. Research on alloys for room temperatures.
- ▷ (III-V) and (II-VI) compounds doped with Mn, Co, Cr...
- ▷ $(\text{Ga}_{1-x}, \text{Mn}_x)\text{As}$: Mn provides spin and polarize hole spin.
- ▷ $(\text{Zn}_{1-x}, \text{Co}_x)\text{O}$: Co provides spin and polarize electron spin.
- ▷ High doping concentration: up to 15 % (vs. $\sim 0,001$ %).

Transition temperatures

- ▷ GaAs: 170 K
- ▷ ZnO: 350 K
- ▷ GaN: 450 K
- ▷ Si: 130 K
- ▷ C: 490 K



Spintronic devices



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Hypothesis and Objectives

Hypothesis

- ▷ Is it possible to simulate the electrical response of spintronic devices using the techniques of electronics?
- ▷ Is the drift-diffusion model still valid for the transport of the spin?

Objectives

- ▷ Create a set of tools to simulate basic spintronic devices.
- ▷ Simulate the diode and tunnel barrier and check with experiment if possible.

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Simulation strategy

Simulation problems

- ▷ Heavily doped materials. Is drift-diffusion model not valid?
- ▷ Quantum-mechanical tunnel transport.
- ▷ Interfaces between different materials.
- ▷ Spin polarization. How it affects to the models?
- ▷ Exotic materials as semiconductors: $(\text{Ga,Mn})\text{As}$, $(\text{Zn,Co})\text{O}$

Solutions

- ▷ Drift-diffusion can be still valid. Correction factors!
- ▷ Non-local tunnel recombination.
- ▷ Graded junctions and thermionic emission model.
- ▷ Zeeman effect: Energy band splitting.
- ▷ Property parametrizing. Literature survey.

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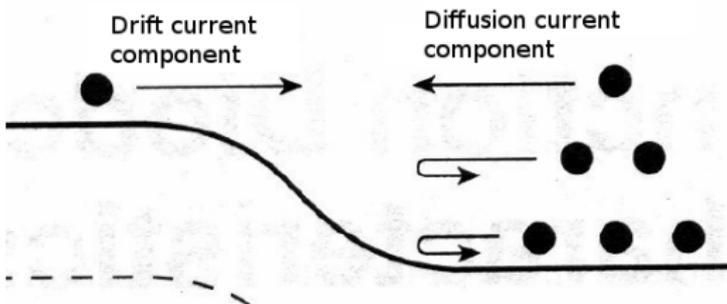
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Drift-diffusion model

Low doped systems

$$\text{Current} = \text{Drift Current} + \text{Diffusion Current} = \alpha n \vec{E} + \beta \frac{dn}{dx}$$



- ▷ Low impurity levels.
- ▷ Low electric fields.
- ▷ Low levels of current.

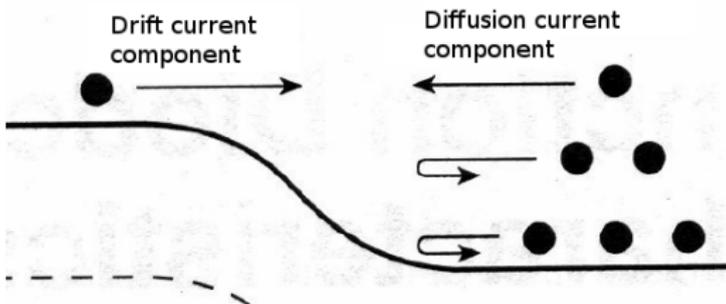
Heavily doped systems

$$\text{Current} = \alpha n (\vec{E} + \vec{E}_{\text{corr}}) + \gamma_{\text{corr}} \beta \frac{dn}{dx} = \alpha n \vec{E} + \gamma_{\text{deg}} \beta \frac{dn}{dx}$$

Drift-diffusion model

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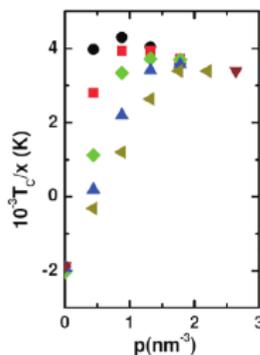
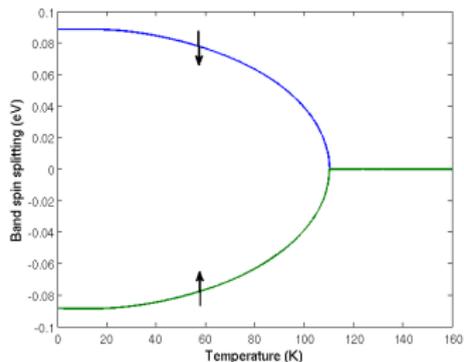
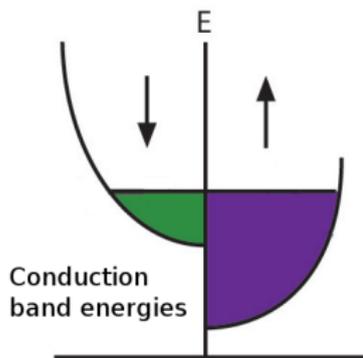


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Zeeman effect: Energy band splitting



- ▷ Spin split bands are created by magnetization in the material.
- ▷ Depends on the impurity magnetic moments and temperature.
- ▷ Critical temperature depends on electron/hole concentration.

Simulator structure

- ▷ 1 dimensional simulator.
- ▷ Finite differences method.
- ▷ Band splitting updated in each iteration.
- ▷ Tunnel recombination for each band.
- ▷ Solve poisson, electron and hole equations:

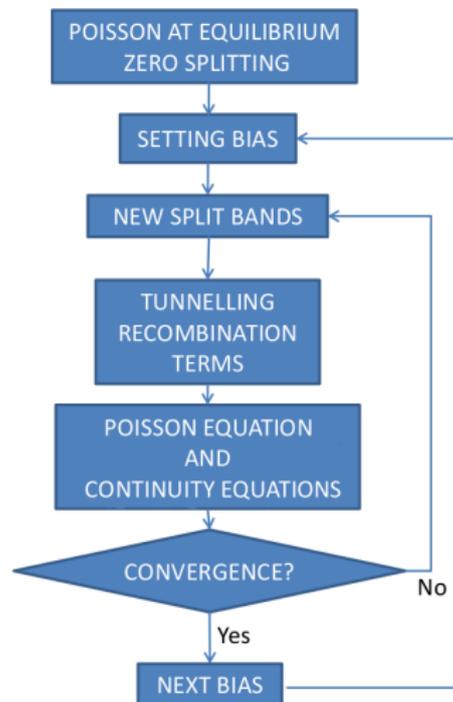
$$\nabla(\epsilon\nabla V) = q_e (p - n + N_D^+ - N_A^-)$$

$$\nabla J_{n\uparrow}^{\rightarrow} = q_e R_{\text{tun}}^{e\uparrow-h\downarrow}$$

$$\nabla J_{n\downarrow}^{\rightarrow} = q_e R_{\text{tun}}^{e\downarrow-h\uparrow}$$

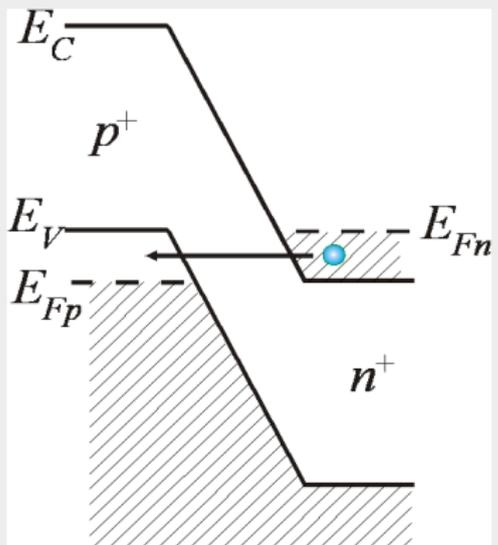
$$\nabla J_{p\uparrow}^{\rightarrow} = -q_e R_{\text{tun}}^{e\downarrow-h\uparrow}$$

$$\nabla J_{p\downarrow}^{\rightarrow} = -q_e R_{\text{tun}}^{e\uparrow-h\downarrow}$$

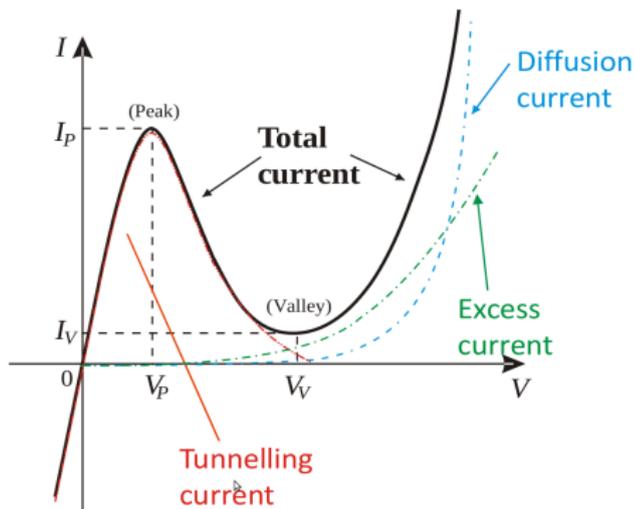


Tunnel diode

Energy bands

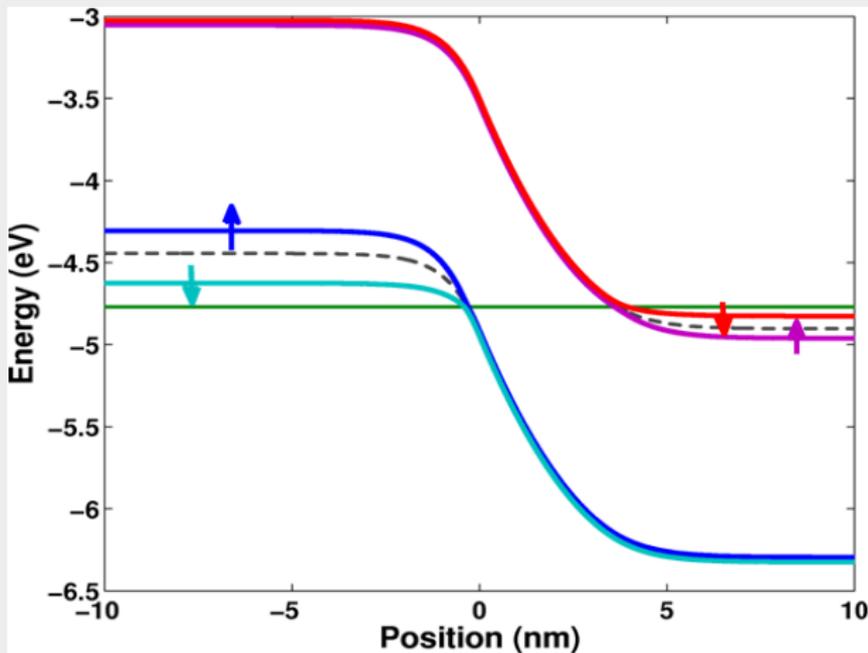


I-V characteristic



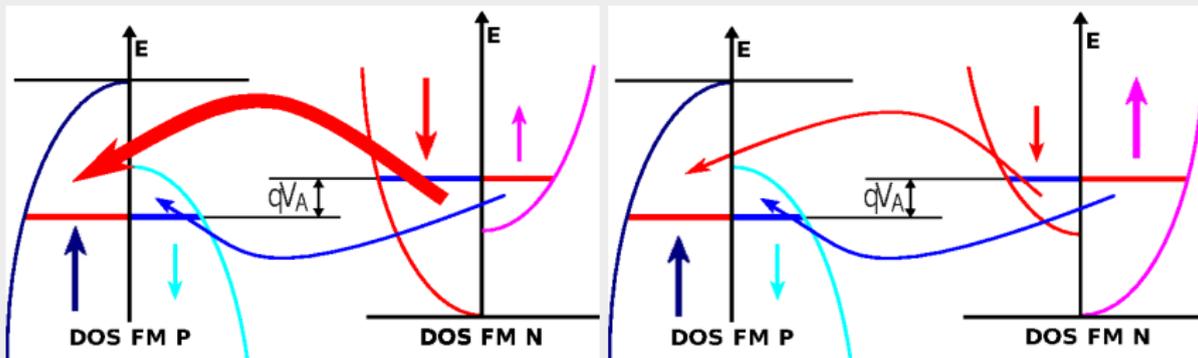
Tunnel diode

Spin split bands



Tunnel diode

Tunnel transport



- ▷ Tunneling recombination reevaluated: $R_{e\uparrow-h\downarrow}$ and $R_{e\downarrow-h\uparrow}$.
- ▷ Tunneling between the majority (minority) bands $I_{ap}(V_A)$.
- ▷ Tunneling between majority and minority bands $I_p(V_A)$.
- ▷
$$\text{TMR}(V) = \frac{|I_p(V) - I_{ap}(V)|}{I_p(V) + I_{ap}(V)} \times 100 \%$$

Tunnel barrier

Structure schematic

Ohmic Contact

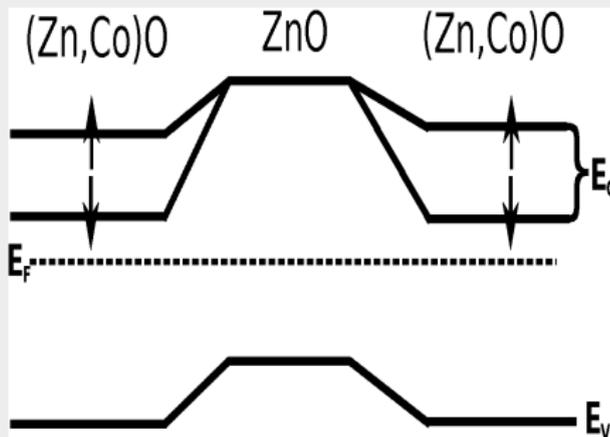
(Zn,Co)O (25 nm)

ZnO (4 nm)

(Zn,Co)O (50 nm)

Ohmic Contact

Spin split bands

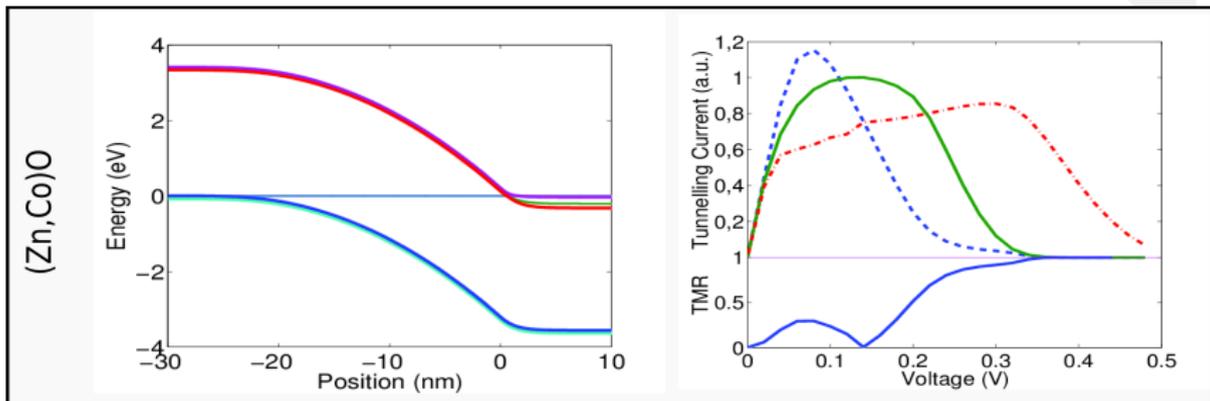
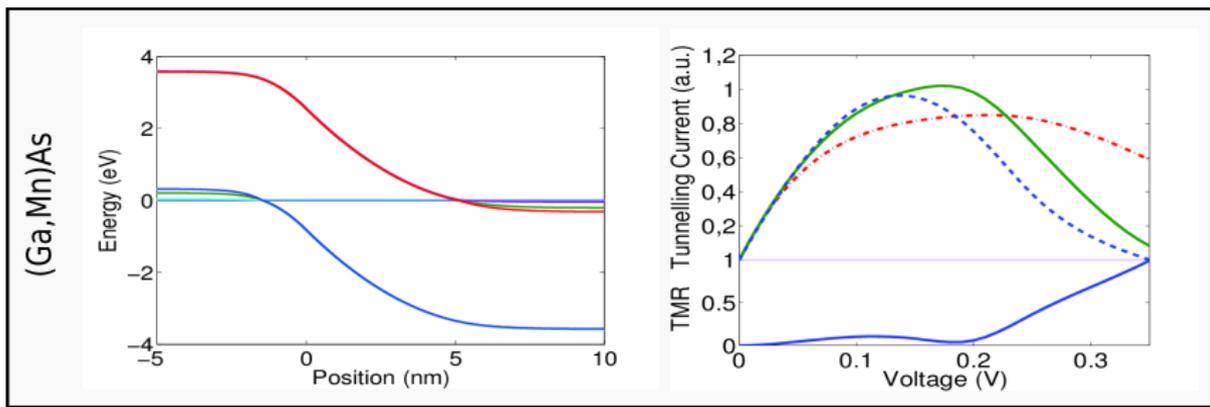


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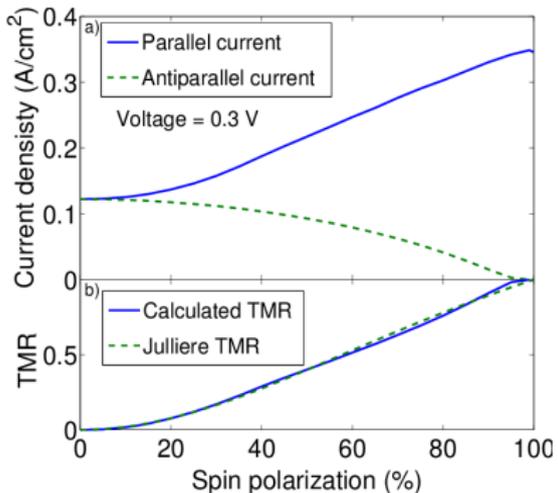
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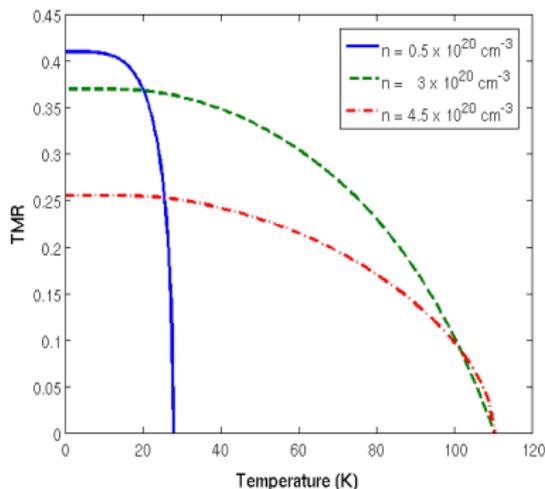
Tunnel diode results



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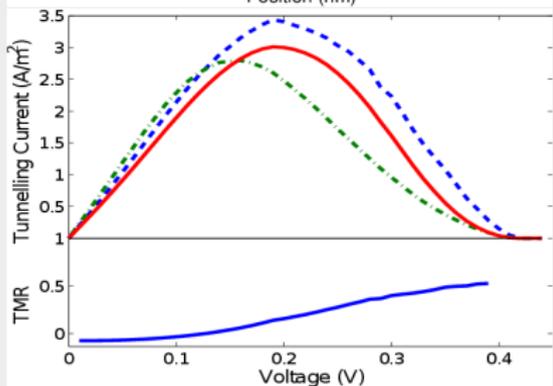
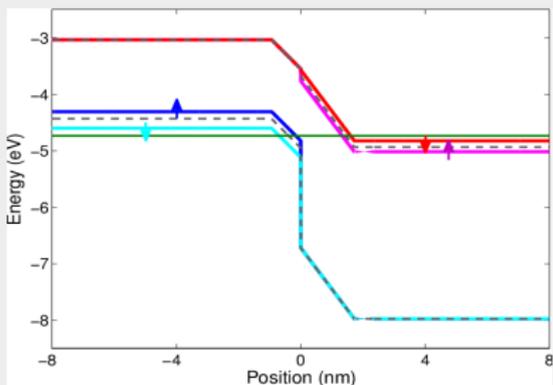
$$\text{Julliere TMR} = \frac{2 \times P_{\text{left}} \times P_{\text{right}}}{1 + P_{\text{left}} \times P_{\text{right}}}$$



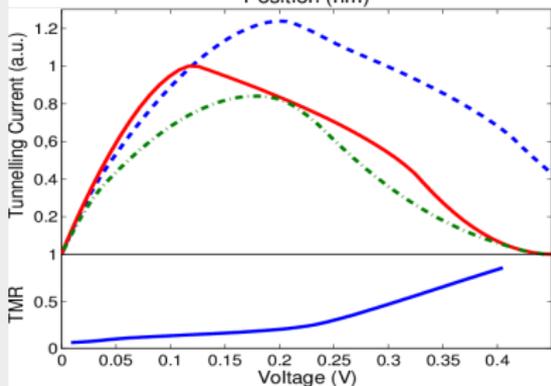
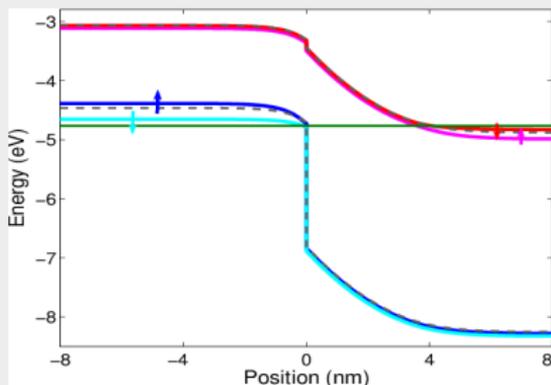
$$\text{TMR} \propto (T_C^\alpha - T^\alpha)$$

Tunnel hetero-diode results

Analytical model

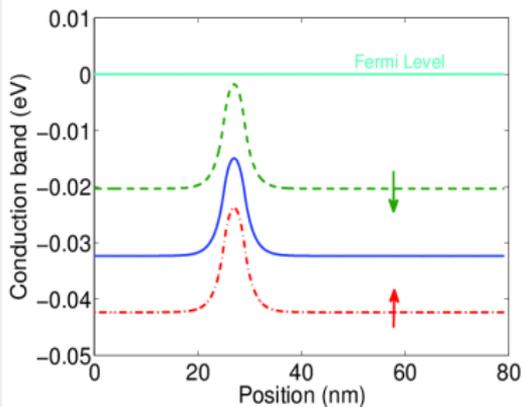


Numerical simulation

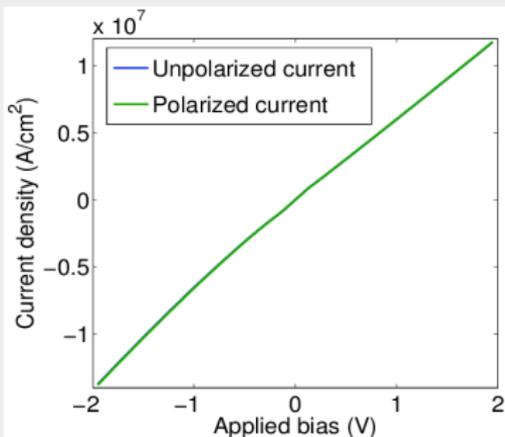


Tunnel barrier results

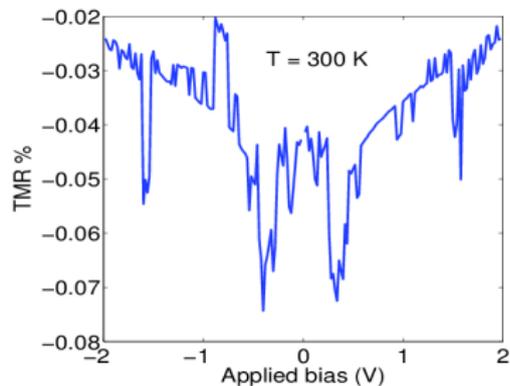
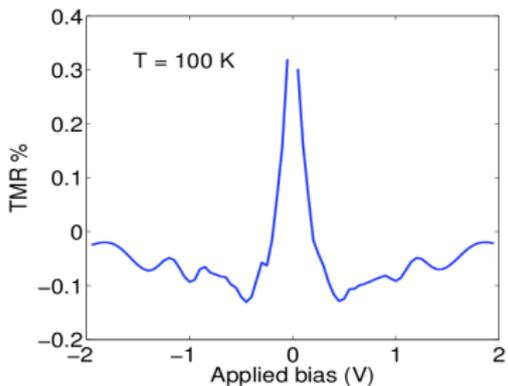
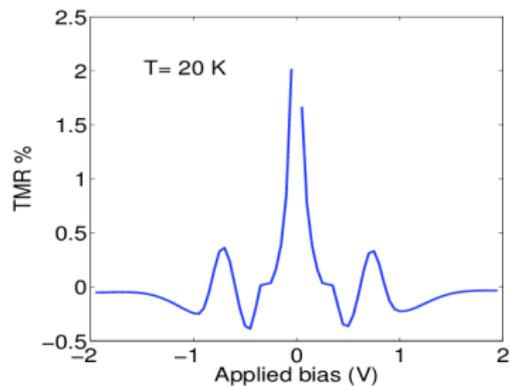
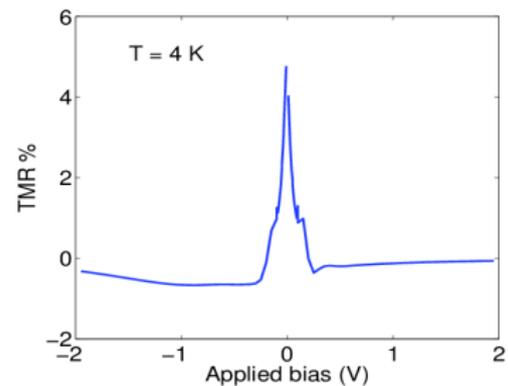
Simulated split bands



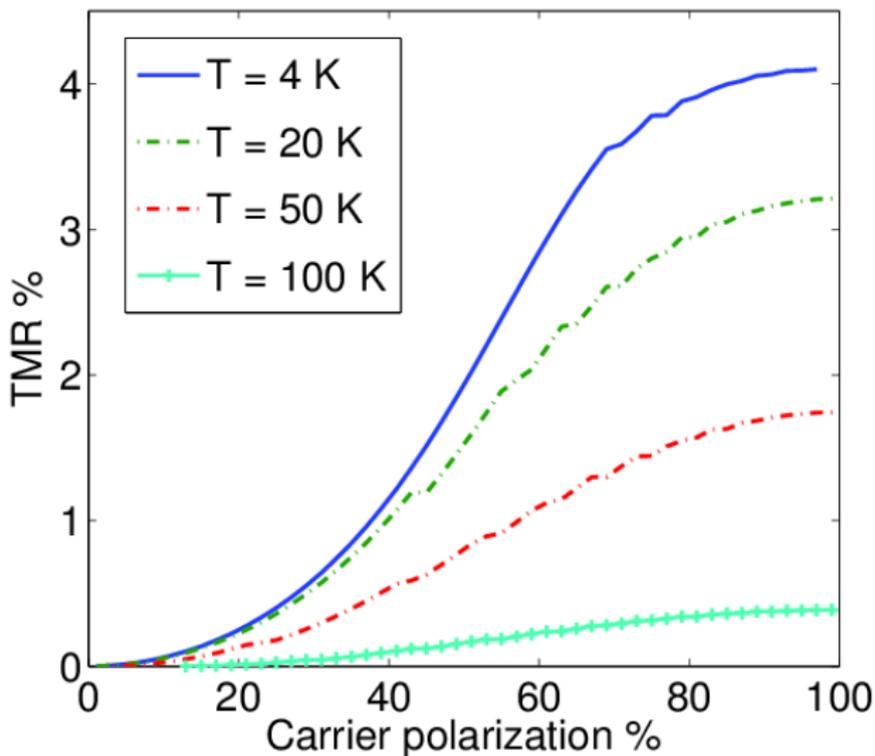
I-V response



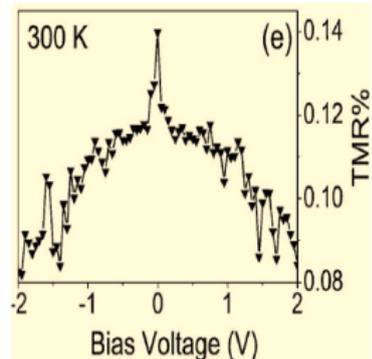
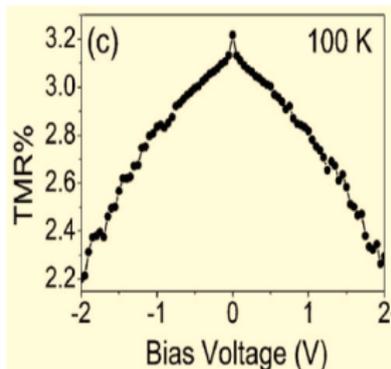
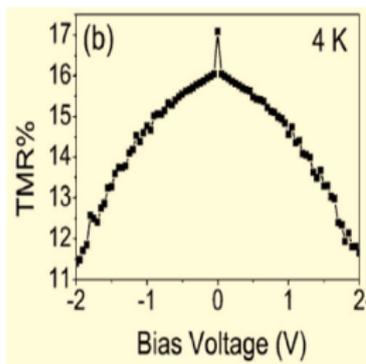
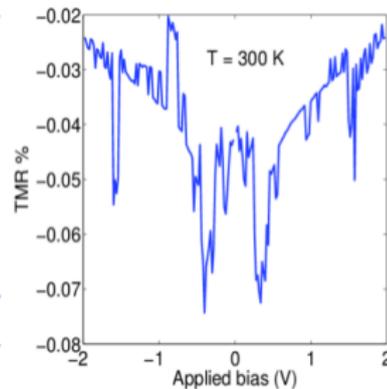
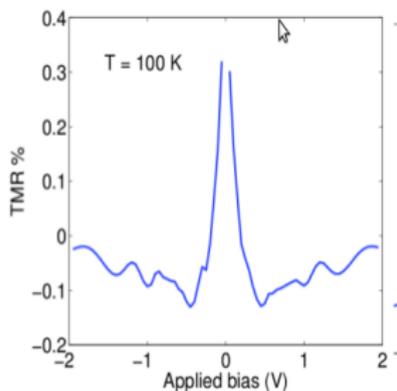
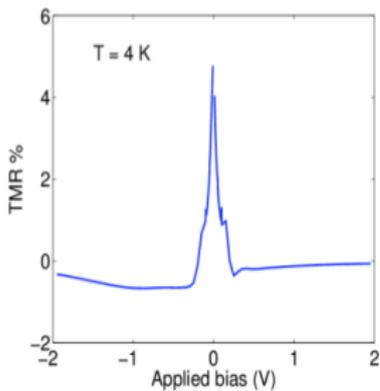
Tunnel barrier results



Tunnel barrier results



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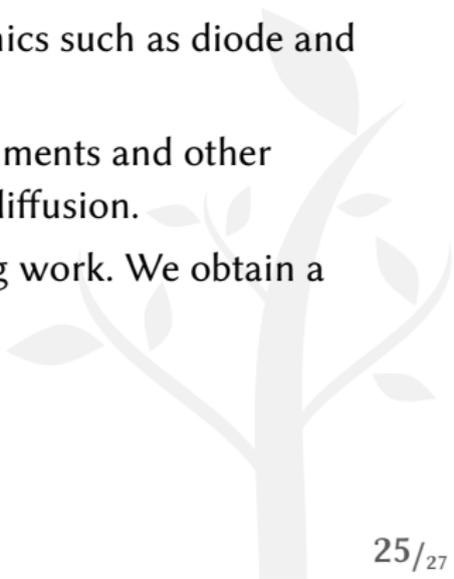
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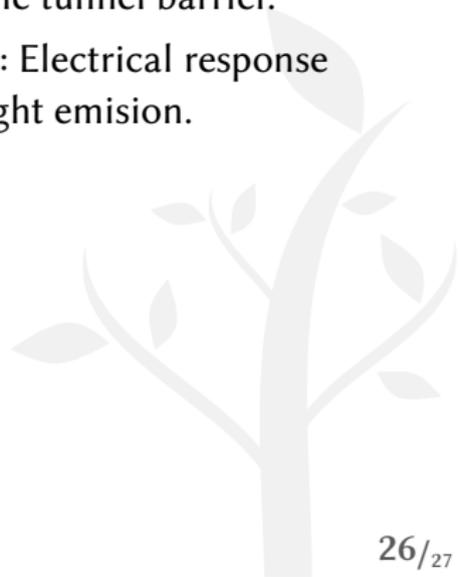
Conclusions

- ▷ We develop analytical and numerical simulators for spin transport using modified drift-diffusion model.
- ▷ Drift-diffusion model offers a non-costly computational model to check hundreds of systems.
- ▷ We analyze to basic structures in the electronics such as diode and tunnel barrier using the TMR figure of merit.
- ▷ Diode results seem to agree with some experiments and other theoretical works when simulated with drift-diffusion.
- ▷ However tunnel barrier needs more modeling work. We obtain a smaller TMR signal than the experiments.



Future work

- ▷ Analyze the behavior of this systems using strongly correlated materials model (Mott materials). Specially the tunnel barrier.
- ▷ Analyze the optical response of the materials: Electrical response under polarized illumination and polarized light emission.



Colaborations

University of Sheffield, UK

Development of suitable models to analyze the ferromagnetic semiconductors.



Host: Prof. Gillian Gehring

University of Swansea, UK

Implementation of the simulator and results checking in Silvaco commercial simulator.



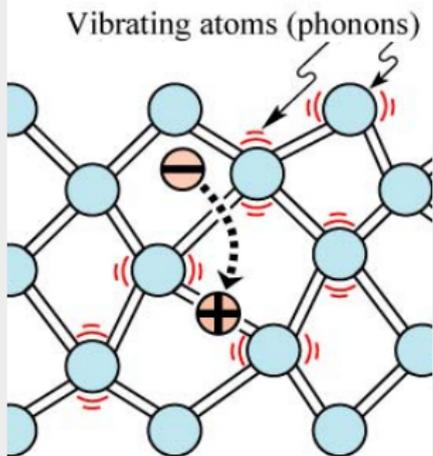
Host: Dr. Karol Kalna

Thank you!
Questions?

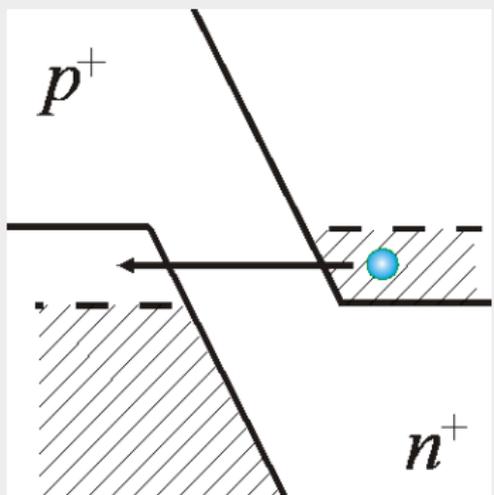


Non-local tunnel recombination

Recombination

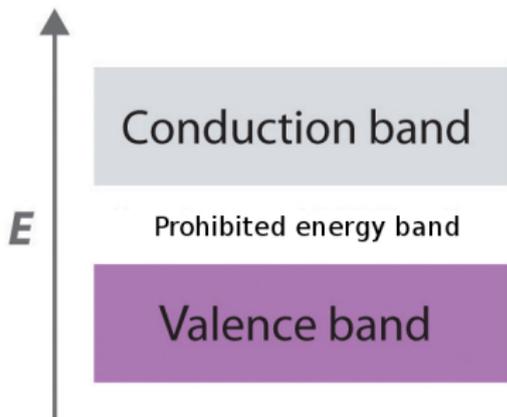
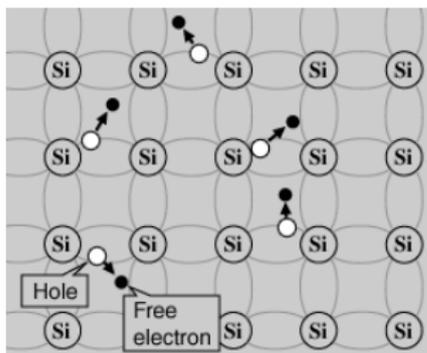


Tunnel Recombination



Tunnel recombination: $R_{\text{tun}} \propto |\vec{E}| \times \Gamma_{\text{tun}} \times T \times D(\epsilon)$

Energy bands



- ▷ Free electrons created from broken bonds between semiconductor atoms.
- ▷ Free electron (negative) move with conduction band energies.
- ▷ Broken bonds (holes, positive) move valence band energies.