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Quantum transport in APAM wires

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Atomic Precision Advanced Manufacturing (APAM)

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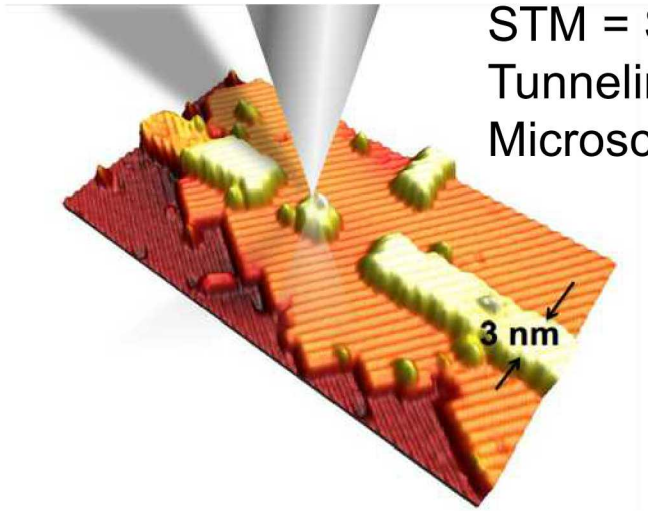
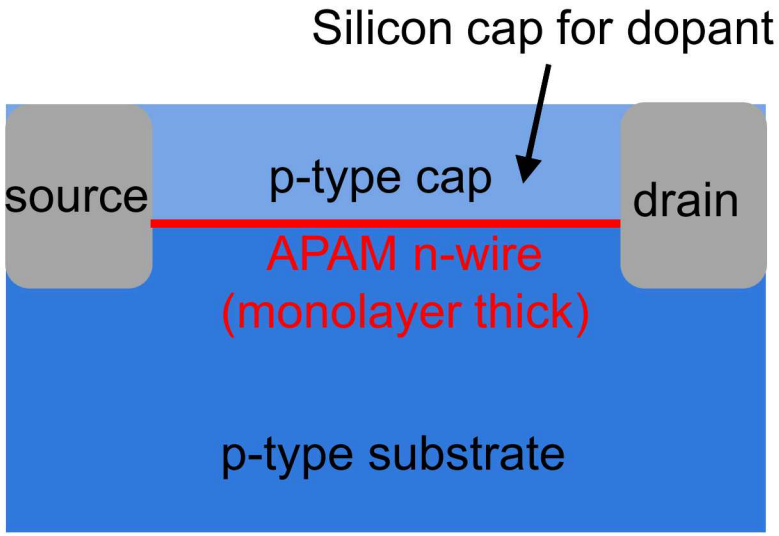
APAM is a process of area-selective dopant incorporation at the atomic scale



STM = Scanning Tunneling Microscope

Example of APAM device



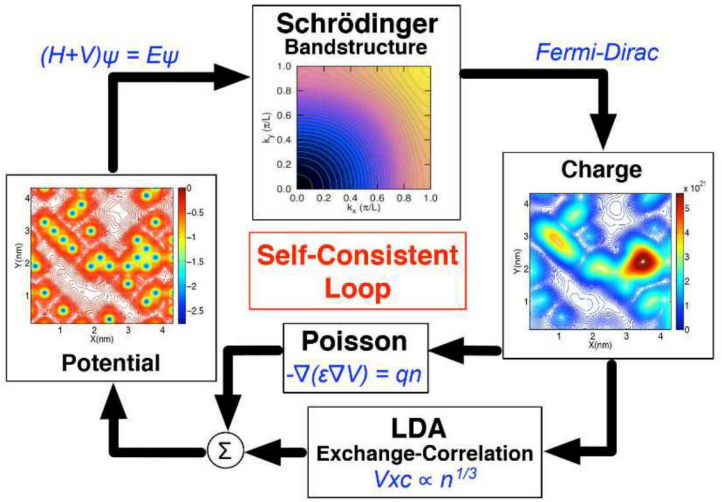
APAM key properties (vs. standard processing)

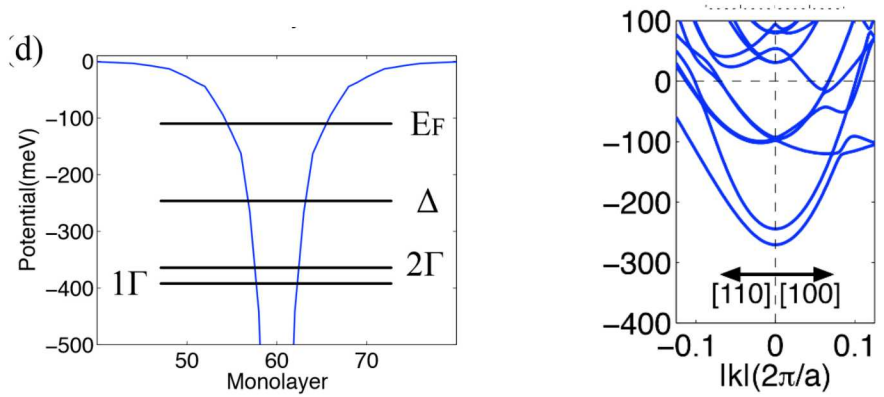
- Atomic precision
- Extremely high density of dopants

APAM can unlock revolutionary opportunities in microelectronics from the atomic physical limit

Previous studies of the C.B. in Si:P δ-layered systems

- Many computational groups attempted to study these systems
- There are many known unresolved contradictions between the theory and experiment
- Gerhard Klimeck's group, world-famous for their quantum transport simulations and tools, spent a significant effort studying Si:P delta-layer systems
- They use "atomistic" tight-binding approach that does take into account valence electrons.
- However, for Si:P-delta systems they did NOT use the open-system treatment, and relied on the closed-system eigenstates (they justified it by considering "equilibrium properties")





"*Equilibrium Bandstructure of a Phosphorus δ-doped Layer in Silicon using a Tight-binding Approach*", Sunhee Lee, Hoon Ryu, Gerhard Klimeck *et al*. (2009)

A recent study revealed the existence of a shallow sub-band!

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The Sub-band Structure of Atomically Sharp Dopant Profiles in Silicon

Federico Mazzola,[1,2] Chin-Yi Chen,[3] Rajib Rahman,[3,4] Xie-Gang Zhu,[5] Craig M. Polley,[6] Thiagarajan Balasubramanian,[6] Phil D. C. King,[2] Philip Hofmann,[7] Jill A. Miwa,[7] and Justin W. Wells[1,*]

[1] *Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway*

[2] *SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, Fife KY16 9SS, UK.*

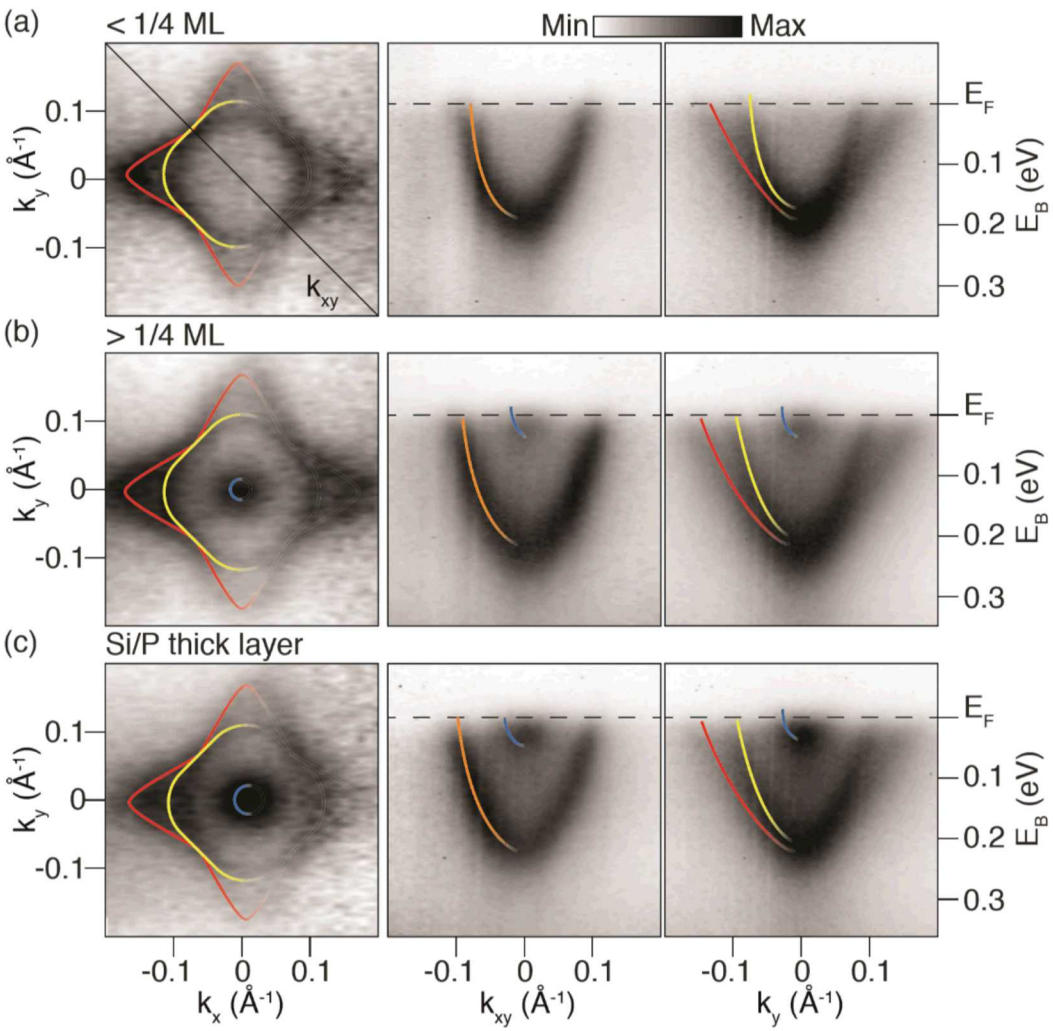
[3] *Department of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, USA*

[4] *School of Physics, The University of New South Wales, Sydney, New South Wales 2052, Australia*

- **ARPES** (angle-resolved-photoemission-spectroscopy) reveals the existence of a **shallow sub-band** (denoted with blue curves) that exists only for relatively high delta-layer values.

The authors

- argue that the majority of current is likely being carried by this sub-band;
- show why this sub-band *cannot* be explained by the traditional theory (e.g. the spin-orbit coupling);
- propose an artificial "solution" by assuming ε~38 for highly-doped Si (T-B)



Quantum transport formalism: a brief reminder

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Density of states: ρ(E) or DOS(E) describes an open quantum system.
Any system with a source-drain is a quantum wire!

The density of states has a functional dependence on energy.

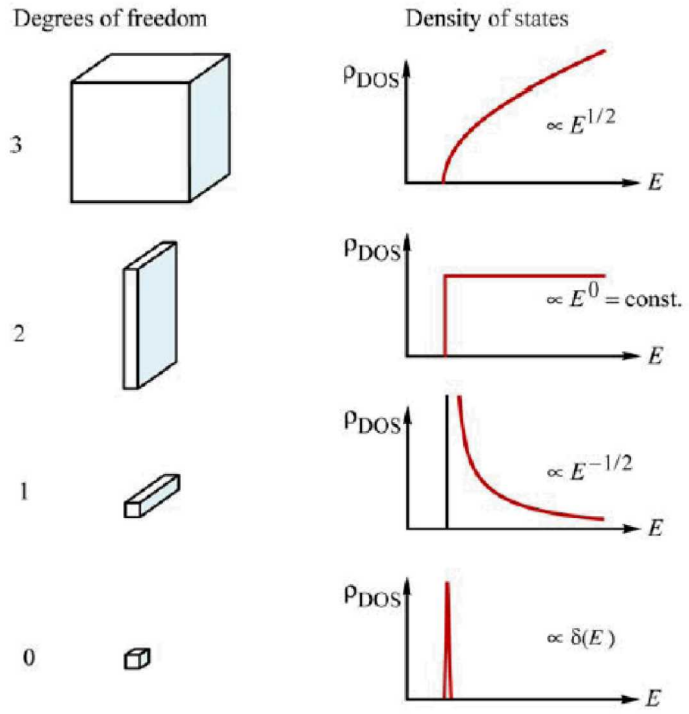


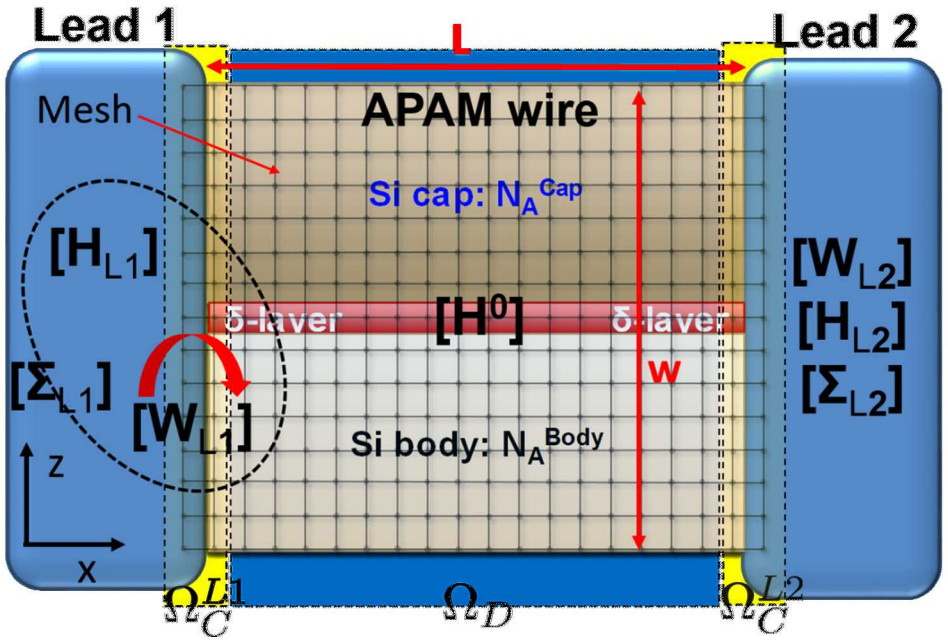
Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

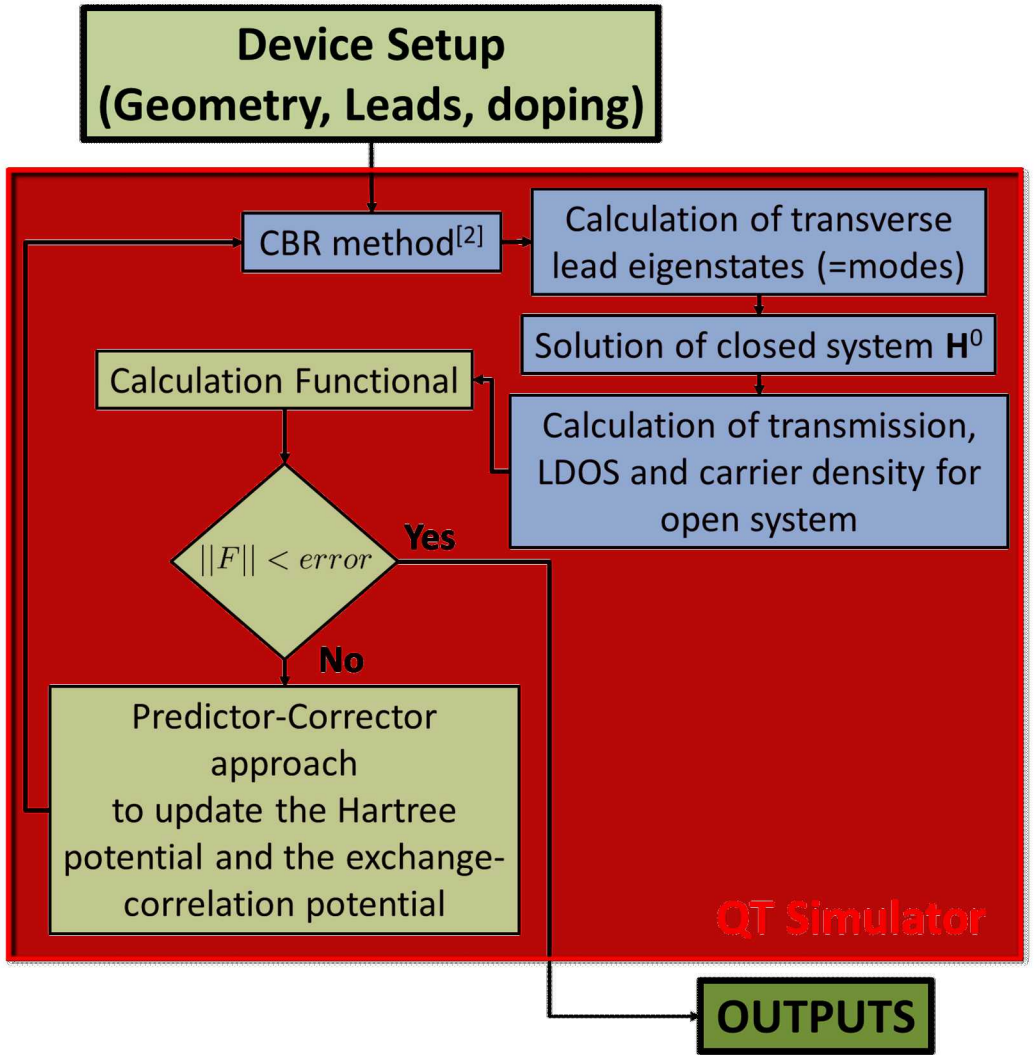
Degrees of freedom	Dispersion (kinetic energy)	Density of states	Effective density of states
3 (bulk)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$	$\rho_{DOS}^{3D} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - E_C}$	$N_c^{3D} = \frac{1}{\sqrt{2}}\left(\frac{m^* kT}{\pi\hbar^2}\right)^{\frac{3}{2}}$
2 (slab)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$	$\rho_{DOS}^{2D} = \frac{m^*}{\pi\hbar^2}\sigma(E - E_C)$	$N_c^{2D} = \frac{m^*}{\pi\hbar^2}kT$
1 (wire)	$E = \frac{\hbar^2}{2m^*}(k_x^2)$	$\rho_{DOS}^{1D} = \frac{m^*}{\pi\hbar}\sqrt{\frac{m^*}{2(E - E_C)}}$	$N_c^{1D} = \sqrt{\frac{m^* kT}{2\pi\hbar^2}}$
0 (box)	–	$\rho_{DOS}^{0D} = 2\delta(E - E_C)$	$N_c^{0D} = 2$

What makes our approach different?

- Simulator to solve quantum transport in **open systems.**
- Fully charge self-consistent solution of Poisson-open system Schrödinger equation.
- Contact Block Reduction (CBR) method.

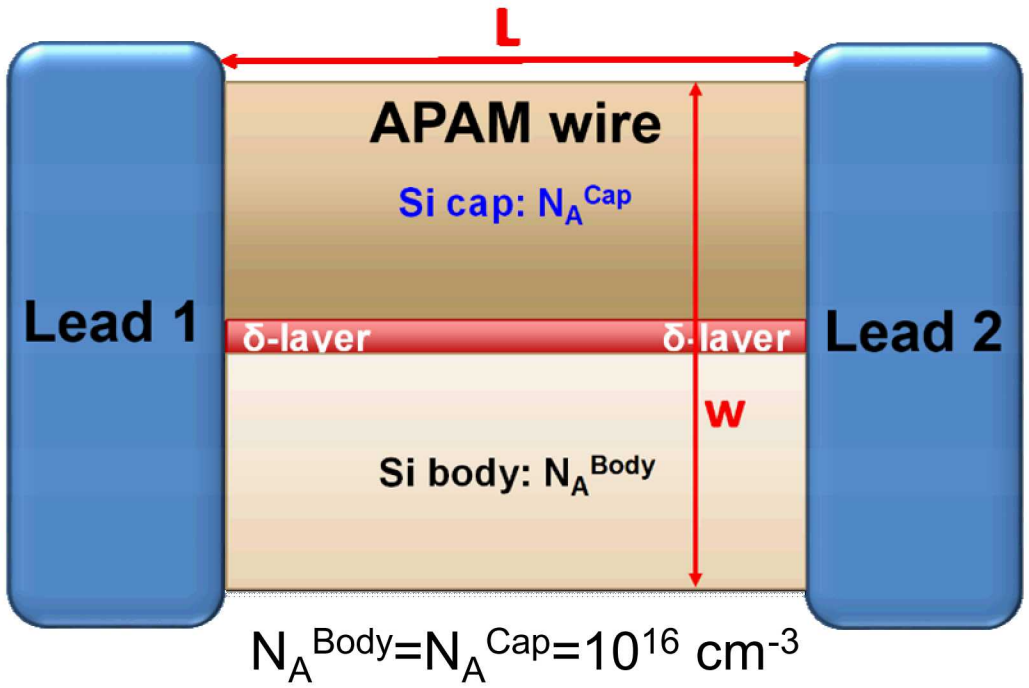
"*Efficient method for the calculation of ballistic quantum transport*", D. Mamaluy, M. Sabathil, and P. Vogl, J. Appl. Phys. 93, 4628 (2003)



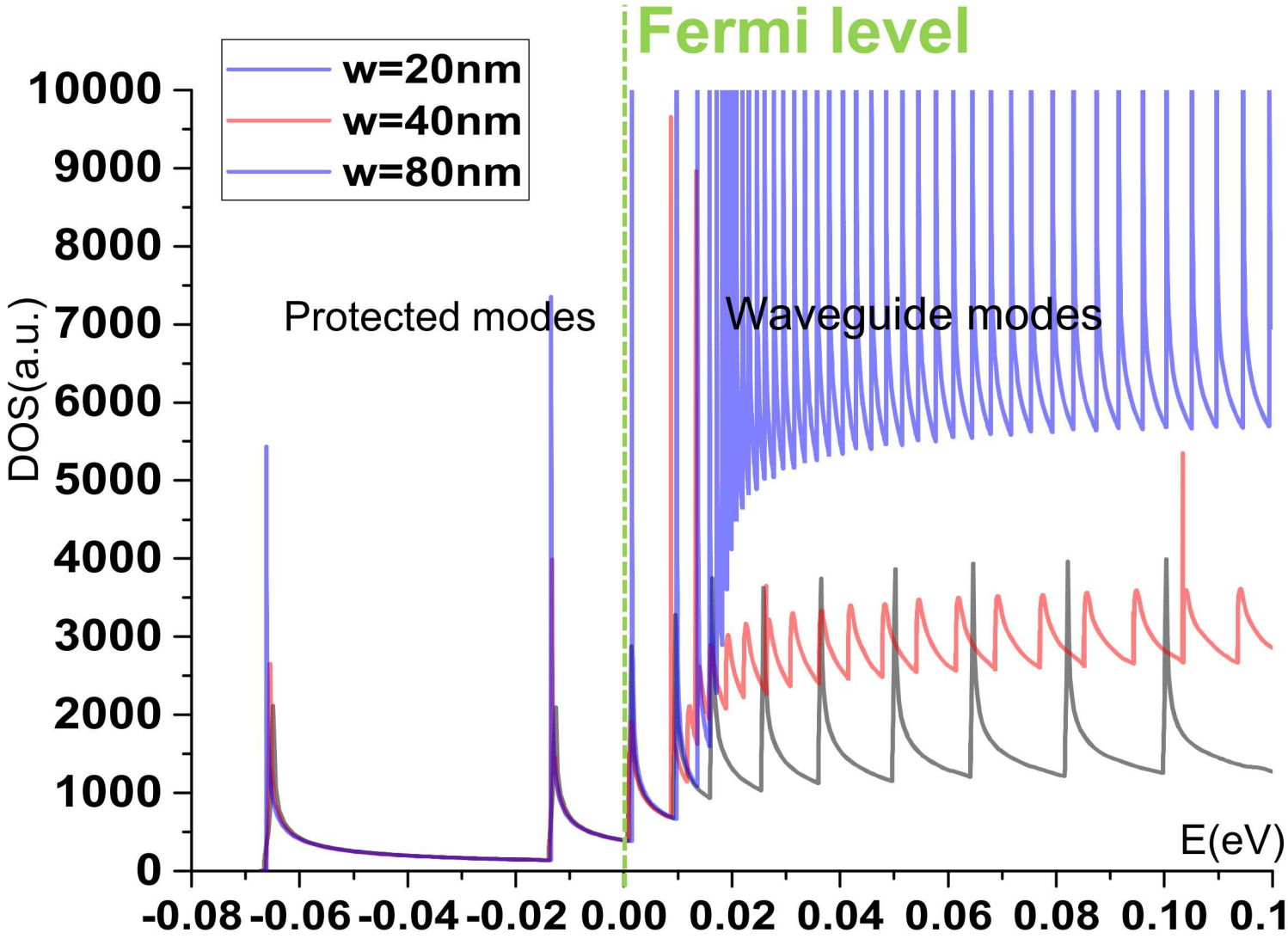


Prediction of a shallow band with unusual DOS

- Below the Fermi level the states are “protected”- i.e. independent of wire geometry.
- Waveguide modes come from conventional confinement, depend on wire geometry.



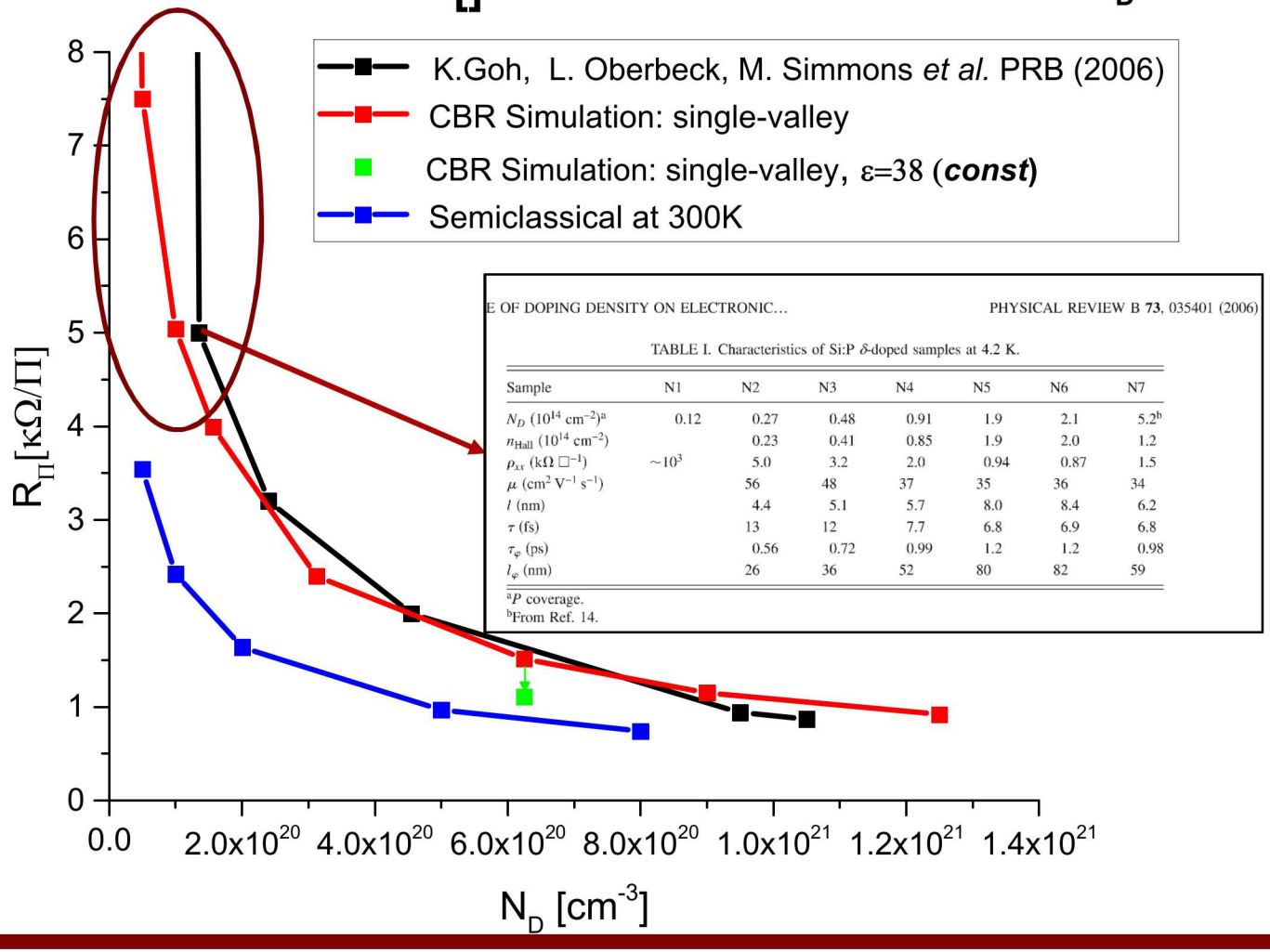
$N_A^{Body}=N_A^{Cap}=10^{16}$ cm^{-3}



Validation: $R_{[]}$ vs N_D, simulation vs measurement

- Accurate everywhere, except for low doping levels.
- A more accurate measurement and a discrete model for simulating impurities are needed in the low doping region.

Sheet resistance $R_{[]}$ vs δ-doping concentration N_D



E OF DOPING DENSITY ON ELECTRONIC… PHYSICAL REVIEW B **73**, 035401 (2006)

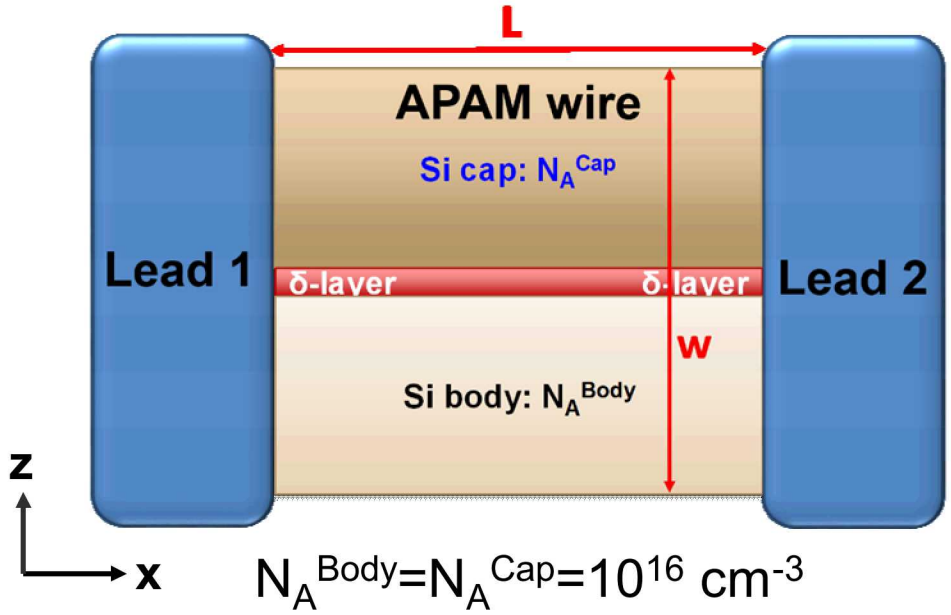
TABLE I. Characteristics of Si:P δ-doped samples at 4.2 K.

Sample	N1	N2	N3	N4	N5	N6	N7
N_D (10^{14} cm^{-2})[a]	0.12	0.27	0.48	0.91	1.9	2.1	5.2[b]
n_{Hall} (10^{14} cm^{-2})		0.23	0.41	0.85	1.9	2.0	1.2
ρ_{xx} (kΩ □$^{-1}$)	~10^3	5.0	3.2	2.0	0.94	0.87	1.5
μ (cm^2 V^{-1} s^{-1})		56	48	37	35	36	34
l (nm)		4.4	5.1	5.7	8.0	8.4	6.2
τ (fs)		13	12	7.7	6.8	6.9	6.8
τ_φ (ps)		0.56	0.72	0.99	1.2	1.2	0.98
l_φ (nm)		26	36	52	80	82	59

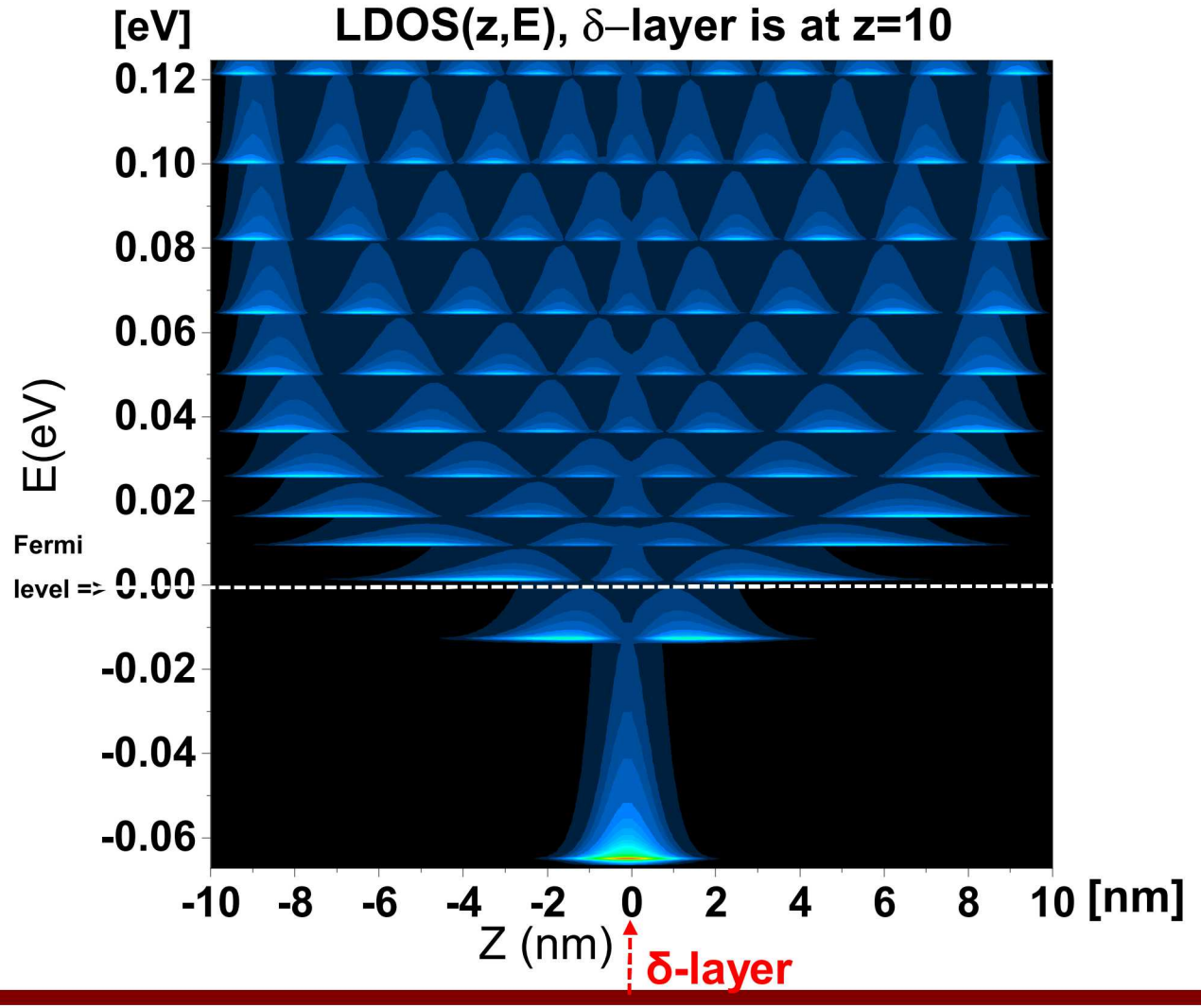
[a]*P* coverage.
[b]From Ref. 14.

LDOS in delta-layer systems: “Quantum Menorah”

- Below the Fermi level the states are “protected”- i.e. independent of wire geometry.
- Waveguide modes come from conventional confinement, depend on wire geometry.



$N_A^{Body}=N_A^{Cap}=10^{16}$ cm^{-3}



Evolution of LDOS for different wire Width

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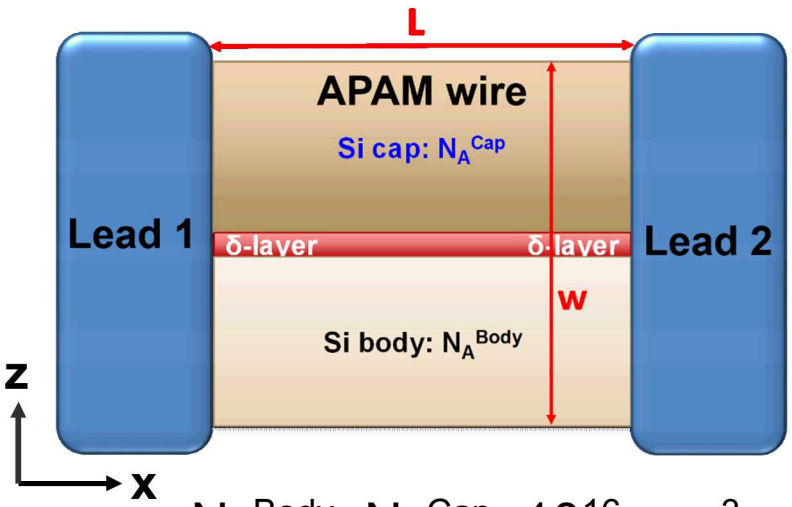
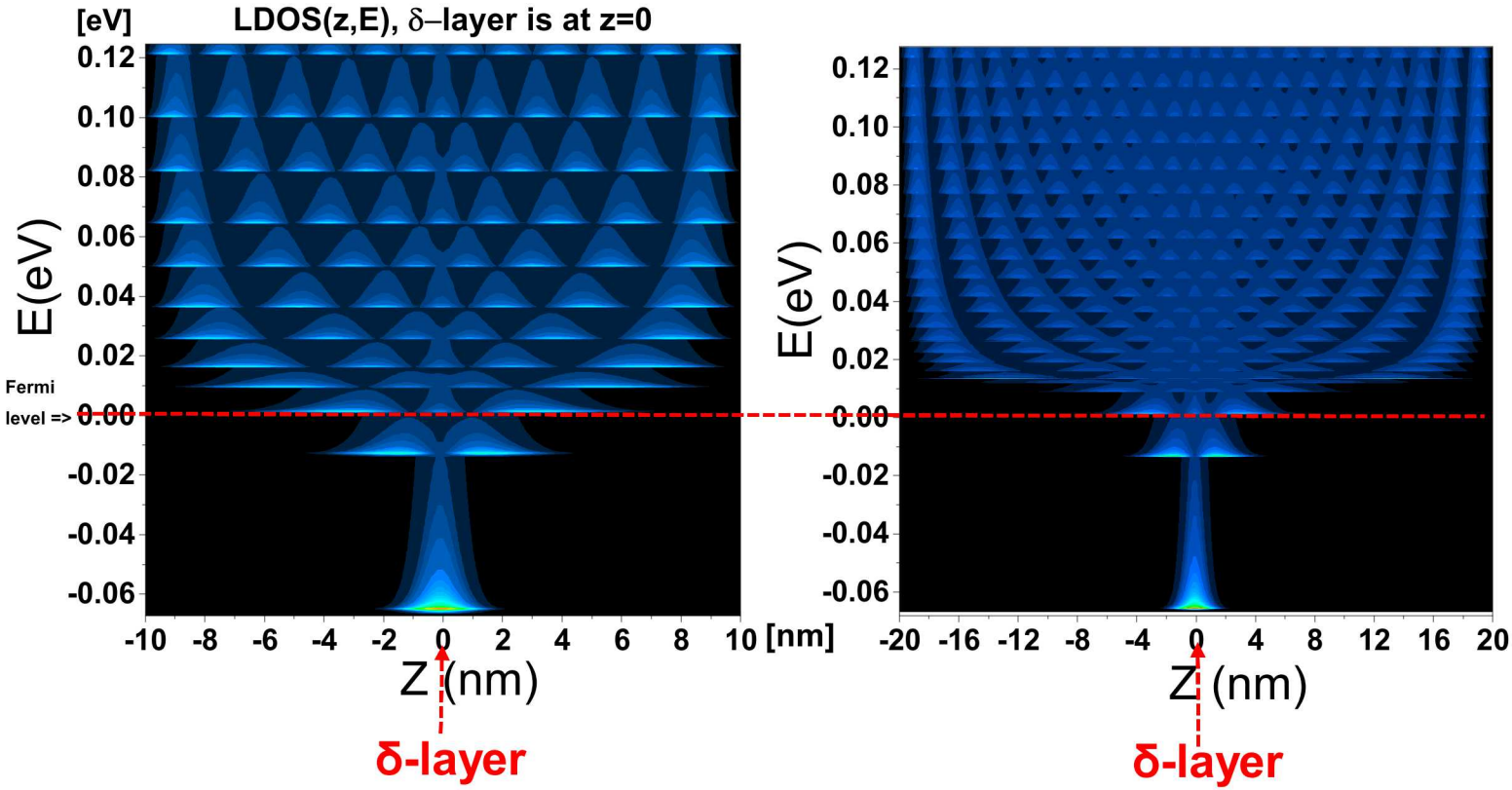
- The protected states do not change with the wire geometry
- Waveguide modes come from conventional confinement, strongly depend on wire geometry.



$N_A^{Body}=N_A^{Cap}=10^{16}$ cm^{-3}

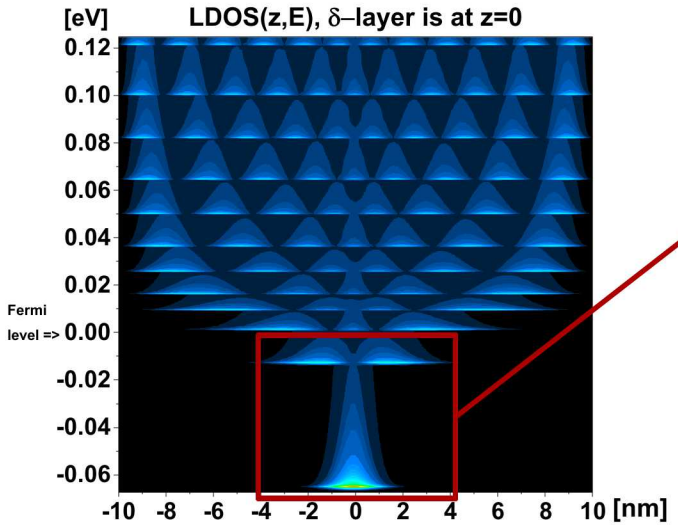
W = 20 nm **W = 40 nm**

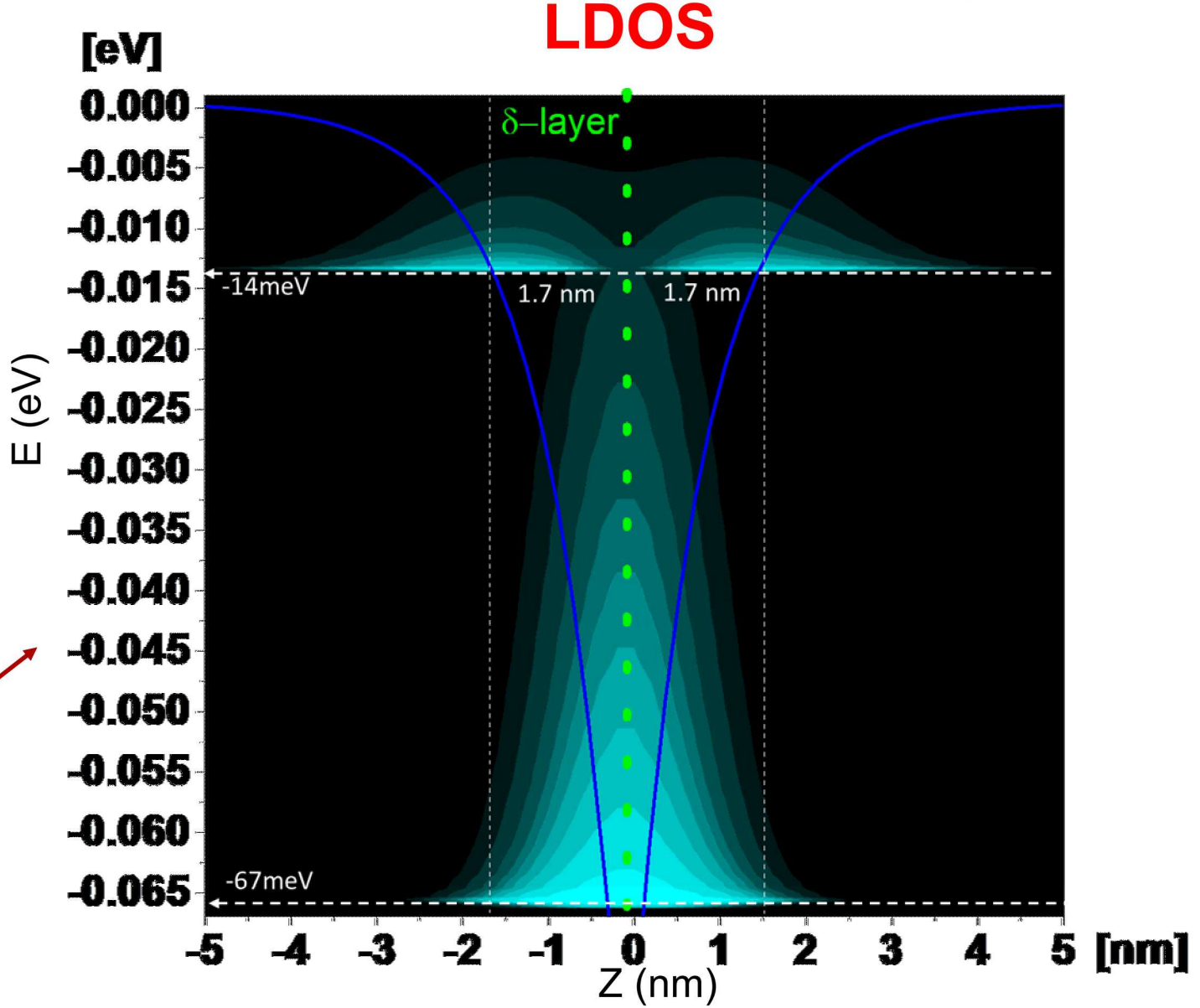


Further analysis shows that by adjusting N_D and N_A one can shift the menorah “up and down” vs the energy scale.

Protected modes due to the delta-layer confinement

- Analysis of LDOS(z,E) reveals the protected modes have distinct structure and energy.
- The two occupied energy levels (-67meV, -14meV) have distinct locations along z-axis (0 and ±1.7nm).

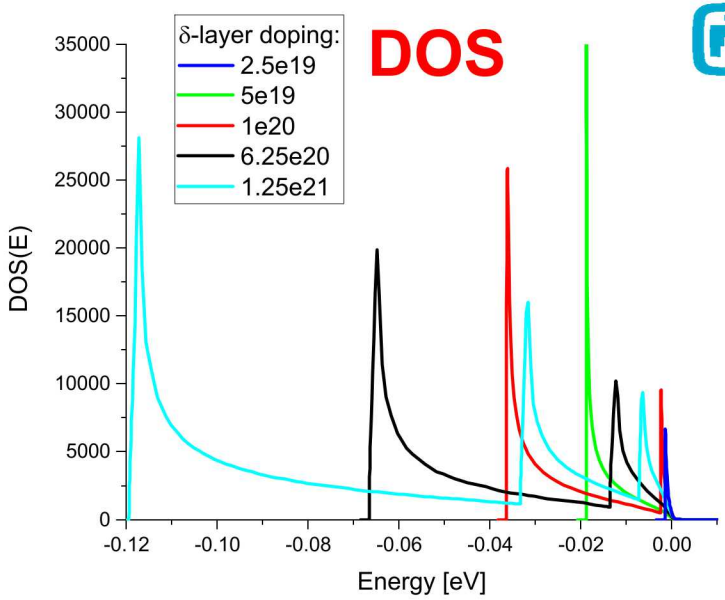


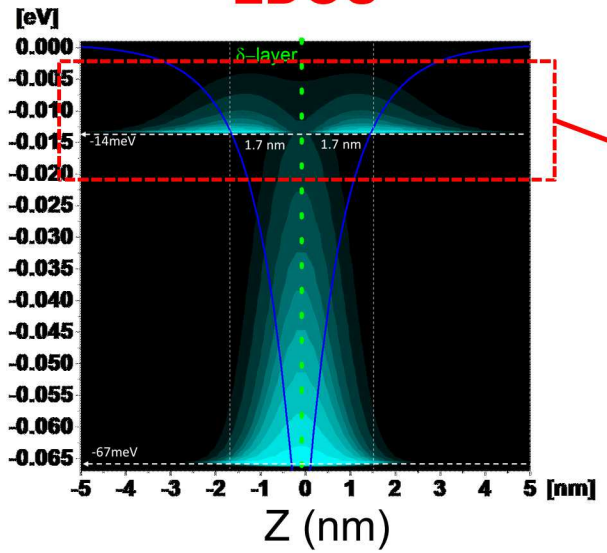


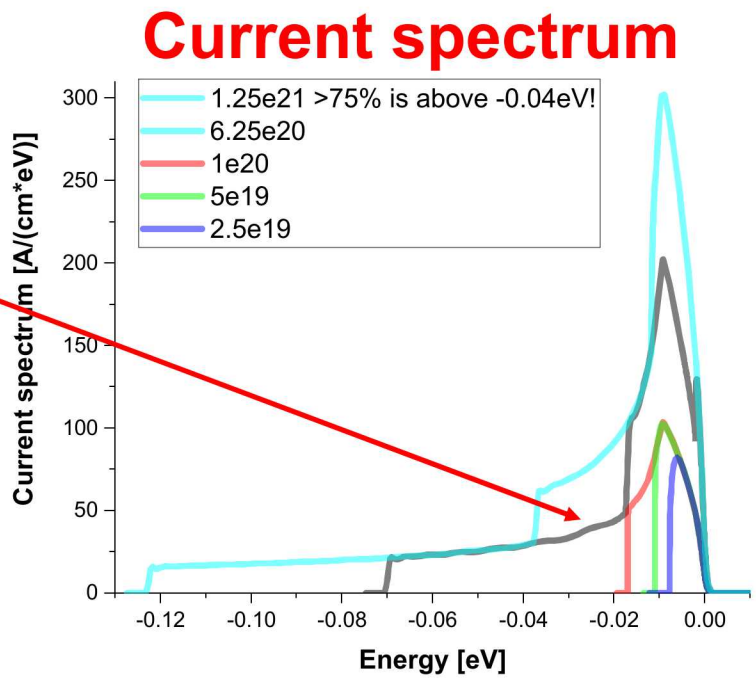
Influence of the δ-doping level

- A first shallow sub-band appears at a doping level around $2x10^{19}/cm^3$. More sub-bands appear as the doping increases. The separation in energy between sub-bands increases with the doping.
- The majority of the current is mainly carried by the electrons with higher energy, corresponding to the sub-band(s) near to the Fermi level, as described by Mazzola *et al.* (2019).

We predict that the higher energy electrons are located ~2nm left and right from the lower energy electrons centered around the delta-layer.







Summary

- We have conducted a fully **open-system** quantum-mechanical study of highly conductive Si:P δ-layered systems
- Unlike previous closed-system studies, our simulations **explains** the existence of a shallow band observed by Mazzola et. al. (2019).
- We **validated** our formalism by **reproducing** Goh et al (2006) the dependence of sheet resistance on the delta-layer doping concentration.
- We predict a special structure of the conduction band in real space, termed "**quantum menorah**". Adjusting N_D and N_A doping levels allows one to transform the "menorah" to achieve a desired level of electron confinement and hence – control the conductive properties of the wire.
- If experimentally confirmed, the existence of a **spatially separated** (~2nm) **free electrons with distinctively different** (~50meV) **energies** could lead to novel applications in energy-filtering, thermo-electronics and digital nanoelectronics.