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Quantum Transport in APAM Wires

Consequences of the novel electronic structure of Si:P δ-layered systems

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Introduction

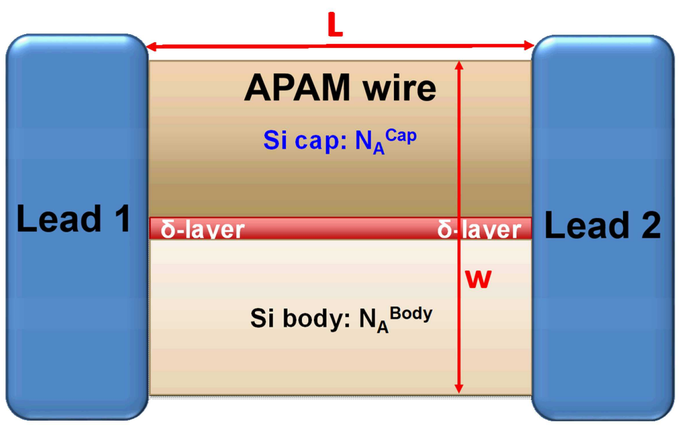
APAM (Atomic Precision Advanced Manufacturing) not only provides atomic-scale control over device structures, but also has unusual material properties originating from the dopants.

Task: The electronic structure of Si:P δ-layered systems is a subject of active research. Recent experiments [1] have discovered an unexpected shallow conduction band feature. Transport current in a device may be dominated by the electrons in this band.

Premise: Quantum-mechanical modeling of electron transport will reveal the consequences of the unusual electronic structure.

Impact: Because allowed modes are determined by the dopants and not wire geometry, electrons are bound tightly enough to be less sensitive to neighboring disorder (e.g. in interfaces).

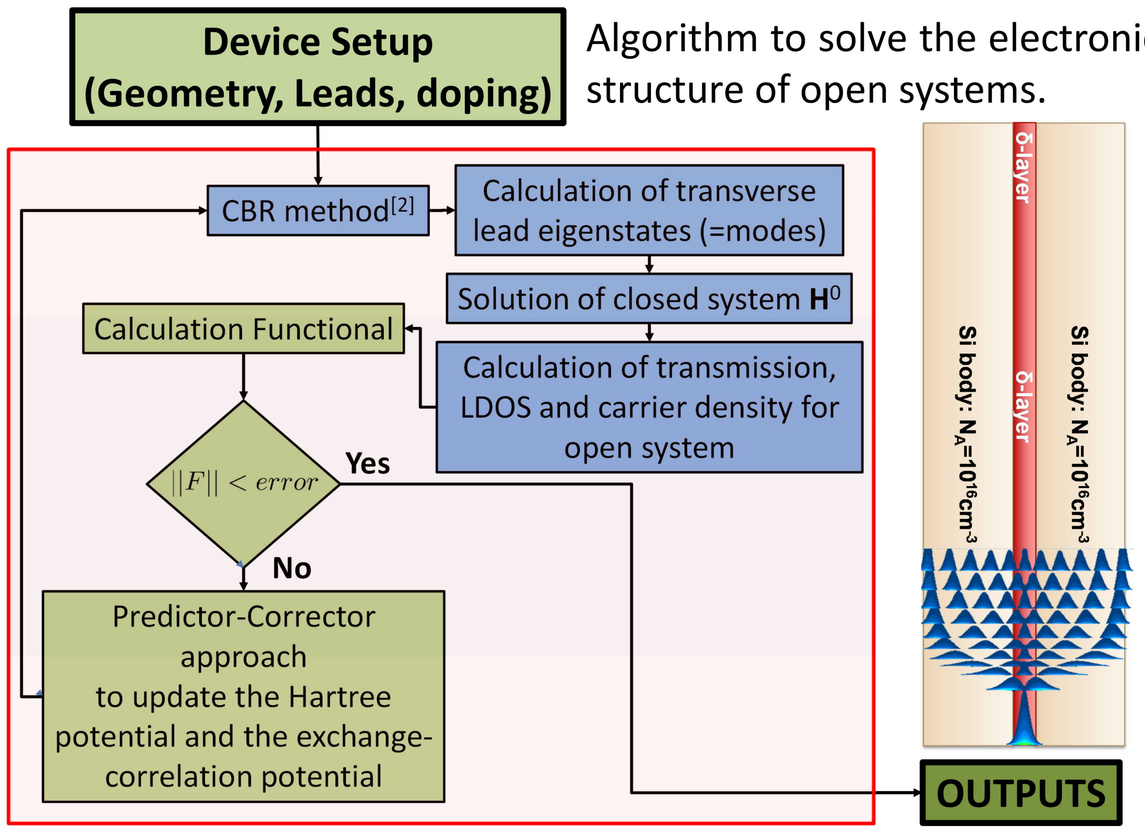
Methodology



Schematic model of a two-terminal APAM wire.

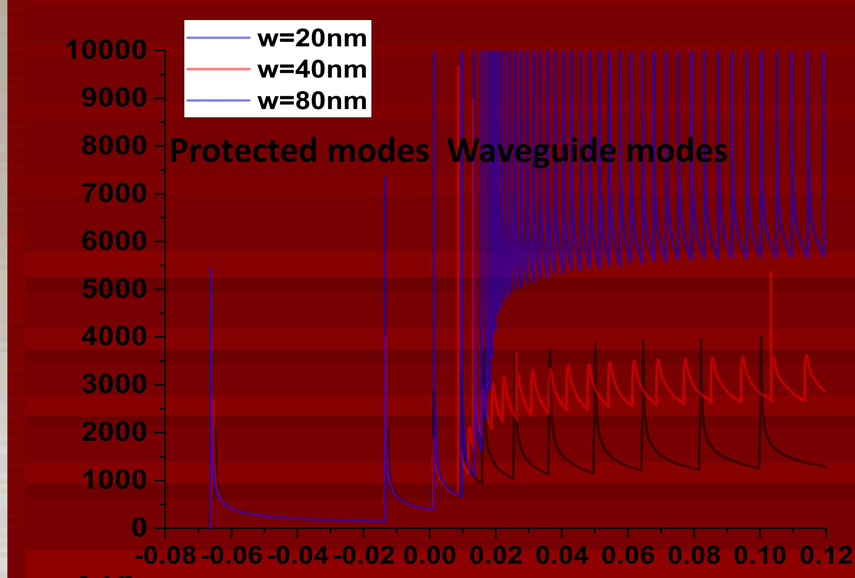
We simulate electronic transport through different configurations of APAM wires connected by two leads, using the SNL's Quantum transport simulator.

Quantum transport simulator

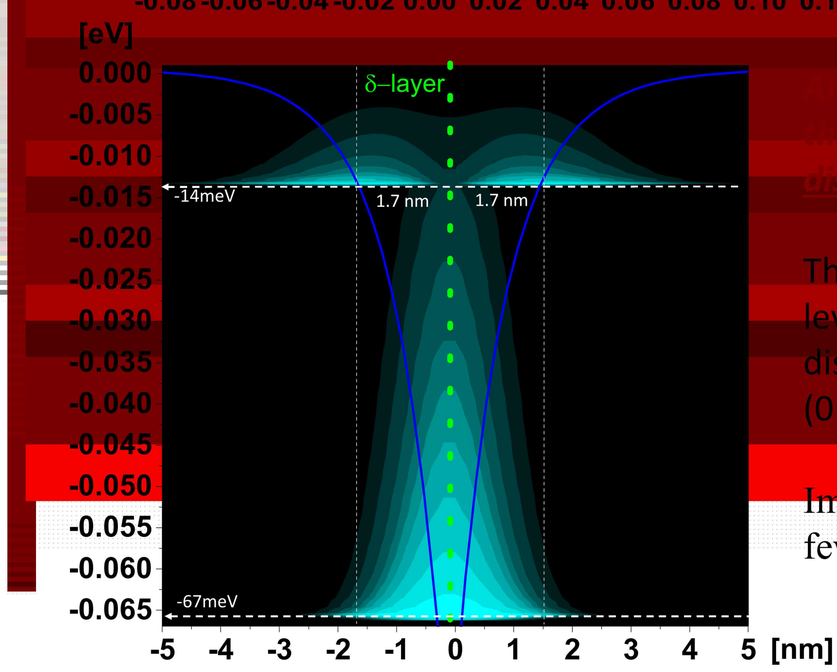


Algorithm to solve the electronic structure of open systems.

Accomplishments



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



The two occupied energy levels (-67meV, -14meV) have distinct locations along z-axis (0 and ±1.7nm).

Implies δ layer can tolerate few nm vertical diffusion.

How can this be used in practice?

If confirmed, confinement from the donor potential in the 'protected modes' appears to be very strong (few nm). APAM δ layer may be more tolerant to diffusion than assumed, while also being robust to interface roughness and impurities past that length scale.

Future Directions

Quantum simulation itself

- Keep identifying situations where quantum simulation is necessary
- Decide where 3D simulation is needed vs. 2D is enough
- Adjust 3D code to work on high performance computers.

Device structures

- Increase complexity : add gates, well implants, complex channels
- Increase understanding : Impurities/ defects, interfaces

[1] F. Mazzola, C.Y. Chen *et al.* https://arxiv.org/pdf/1904.10929.pdf.
[2] D. Mamaluy, X. Gao, APL 106, 193503 (2015).

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NNSA National Nuclear Security Administration

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