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Shizuoka University

Research Institute of Electronics

Nanodevices Lab. Research Institute of Electronics

First-principles study of bandgap electronic states under electric field in Silicon nanowires with discrete dopants

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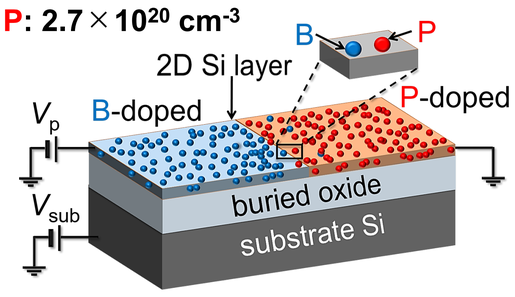
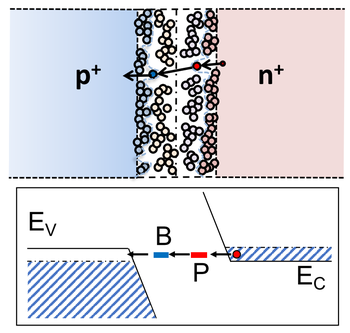
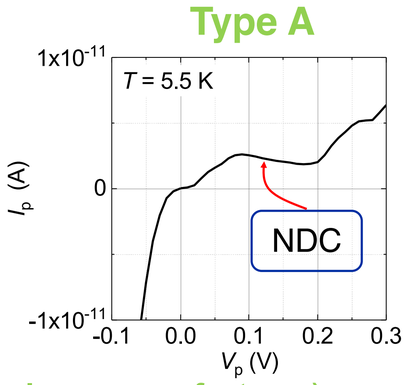
Introduction – low-dimensional silicon *pn* tunnel diodes

B: 0.9×10^{20} cm^{-3}
P: 2.7×10^{20} cm^{-3}

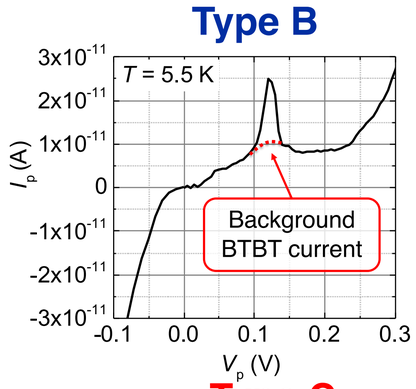




Type A



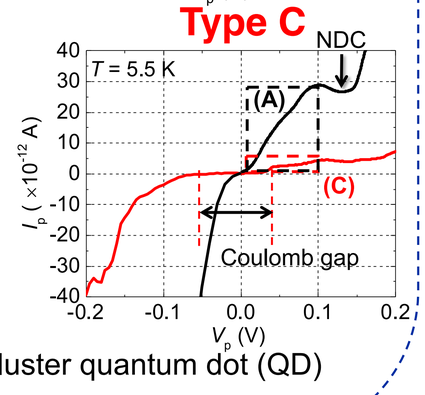
Type B



Type A (only common features)
- 2D Quantization
- Phonon Assistance

Type B (w/ sharply enhanced current peak)
- Band-to-band tunneling (BTBT) via the energy states of a donor-acceptor (D-A) pair
  M. Tabe *et al.,* Appl. Phys. Lett. **108**, 093502 (2016).

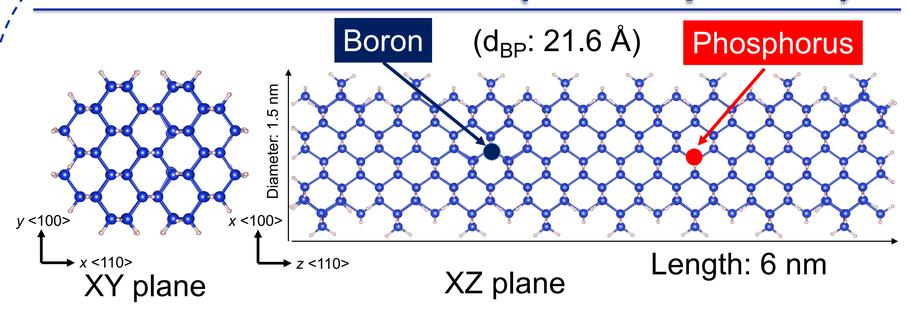
Type C



Type C (w/ Coulomb staircase)
- Prominent low-current gap at low biases
- Single-charge BTBT (SC-BTBT) via dopant-cluster quantum dot (QD)

G. Prabhudesai *et al.,* Appl. Phys. Lett. **114**, 243502 (2019).

Simulation details (DFT: OpenMX)



Distance between P-B : 5.9, 13.5, 21.6, 28.8, 36.5, 44.2 Å

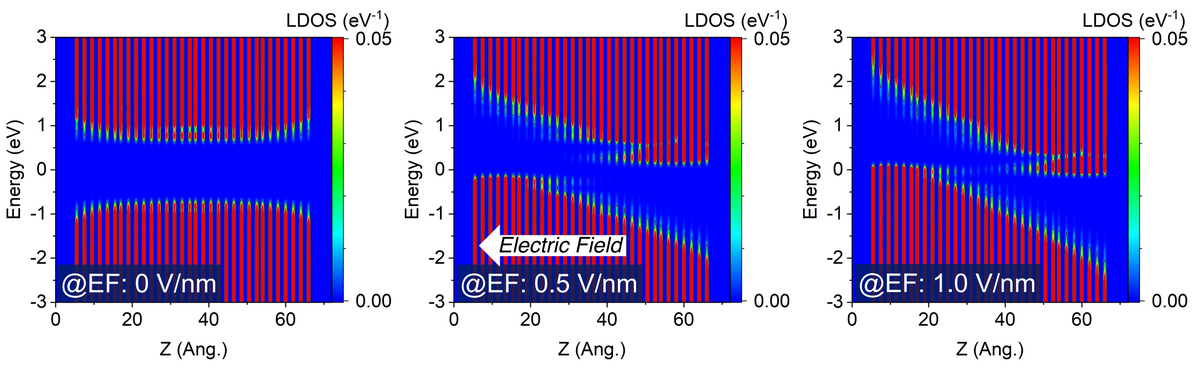
- **Dopants:** inserted substitutionally in a Si nanoplate
- **All dangling bonds:** passivated by hydrogen (H)
- **Geometry optimization**: performed before calculations
- **DOS (density of states)**: calculated under electric field

- **Exchange correlation:** GGA
- **K-point:** 1 × 1 × 1 (gamma point only)
- **Cutoff Energy:** 150 Rydberg
- **Vacuum layer:** 20 Å
- **Convergence criteria (Geometry Opt.):** 10^{-2} eV/Å

Accurate way to investigate the atomic-level effects

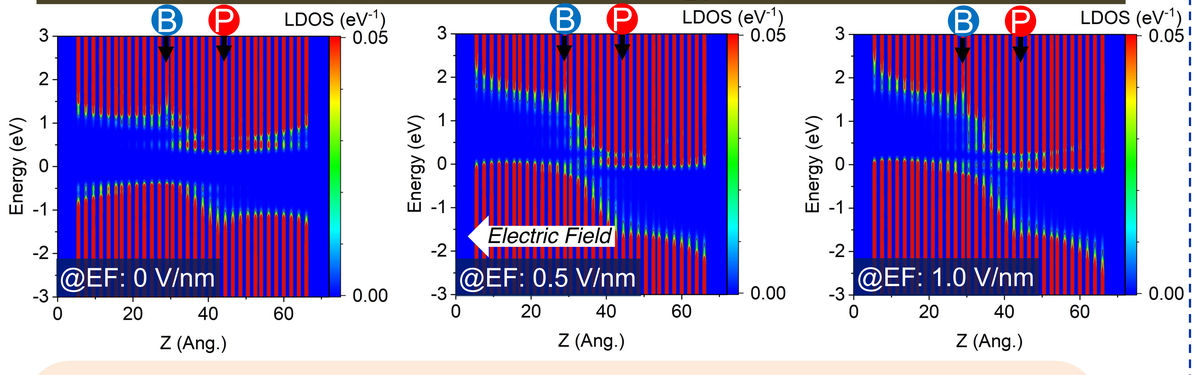
LDOS (Local Density of States)

Non-doped structure



Results:
- The valence and conduction band on the center of nanowire are flat without external field.
- Due to the hydrogen passivation on the surface of the Si nanowire, the band bending is observed around the surface at EF = 0.

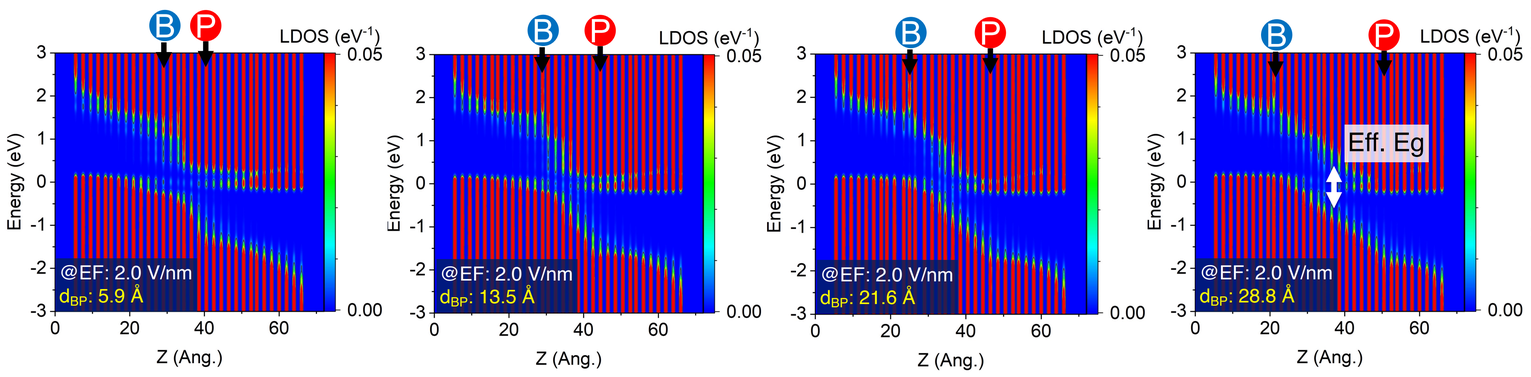
Co-doped structure @ d_{BP} = 21.6 Ang

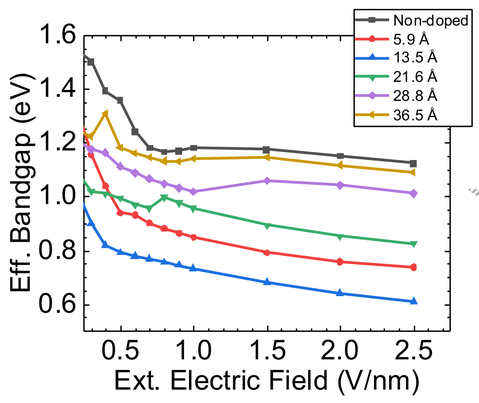


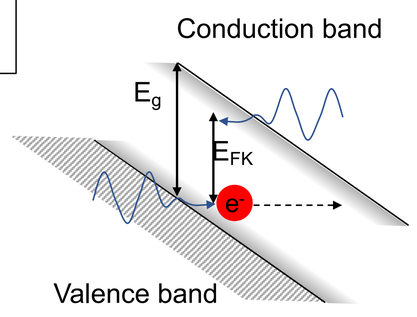
Results:
- The built-in potential occurs without external electric field, because a pair of dopants behave as opposite-polarity point charges.
- Energy states become visible between P and B for electric field >0 V/nm.
- The bandgap is getting smaller around depletion layer, by increasing the electric field.

The effect of even a single P-B pair is significant in modulating the band diagrams

Analysis of bandgap narrowing at high electric field







Results:
- The **edges of the conduction and valence bands** become discontinuous
  → penetration of energy states inside the effective bandgap occurs at specific energies
- There are some difficulties to analyze the effective bandgap below 0.2 V/nm.
- Co-doped and non-doped structure have similar trends of bandgap narrowing by increasing external electric field.

→ The difference of effective bandgap among each P-B pair may be caused by an internal electric field which originated from a P-B.

Franz–Keldysh Effect

When an electric field is applied into semiconductor, the electron and the hole wavefunction penetrates into the bandgap. Thus, E_{FK} becomes smaller than E_g.

Experimental observation on bulk silicon is reported.
→ **Not yet reported in Si nanostructures**
[*]Y. Yacoby, Phys. Rev. **142**, 445 (1966).

Modulations of band edges are sensitive to the P-B pair configuration → likely dependent on the electric field and energy states of the dopants

Conclusions

- **By means of *ab initio* simulations, it is found that an external electric field can assist in enhancing the interaction between a phosphorus (P) atom and a boron (B) atom.**
- **Results suggest that "the bandgap narrowing" can be enhanced for the most suitable dopants' positions and energy levels.**

A donor-acceptor pair can be tuned for band-to-band tunneling applications → Atomic-level *pn* diode