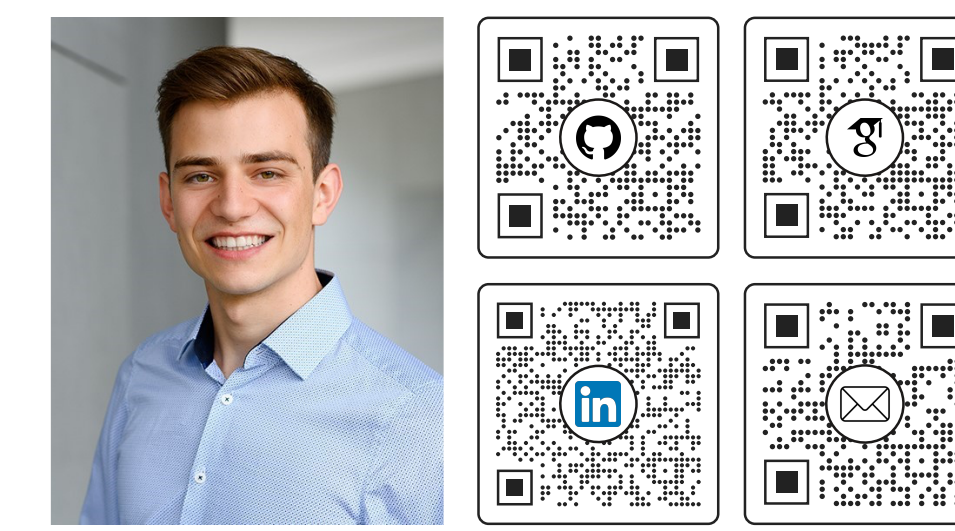


Design and Simulation of Atomic-Scale Computing: Bridging Computer Science, Electrical Engineering, and Physics

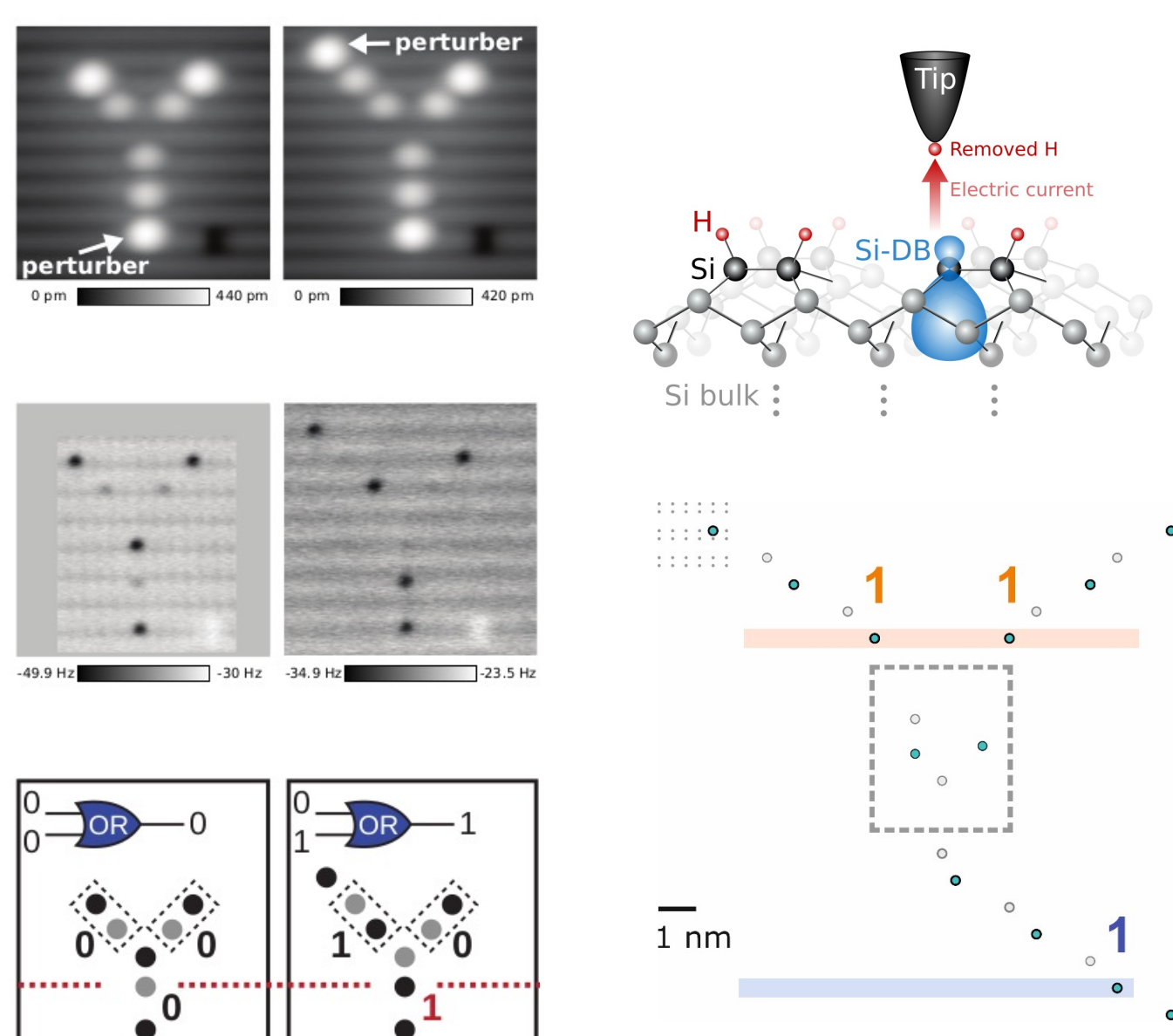
Jan Drewniok, *Supervisor: Robert Wille*



Motivation

The rapid expansion of AI and digital transformation across industries is dramatically reshaping the **demand for computing power**. The **Silicon Dangling Bond (SiDB) technology** represents a leap forward in **energy-efficient computation**, surpassing the limitations of traditional transistor-based designs. Based on single atoms, it enables **atomic-scale computing** by precisely controlling charge states for logic, memory, and logic-in-memory functionality. The SiDB technology has already **entered the commercialization phase**, with companies like *Quantum Silicon Inc.* already applying it to industrial applications.

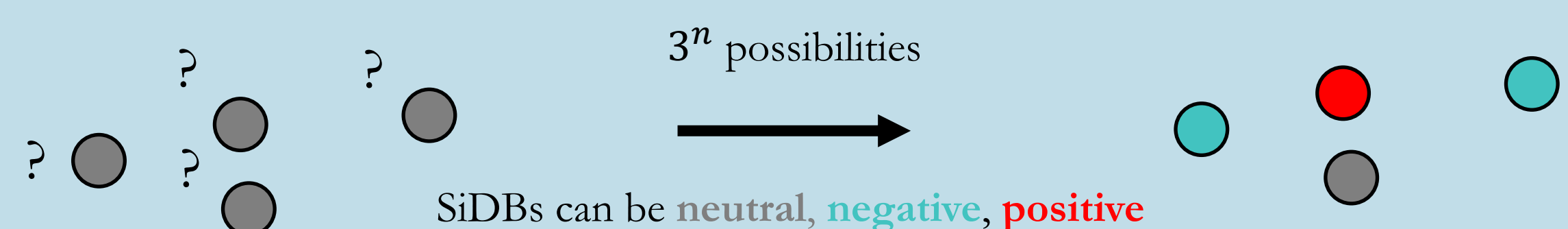
Technology



Thesis Objectives

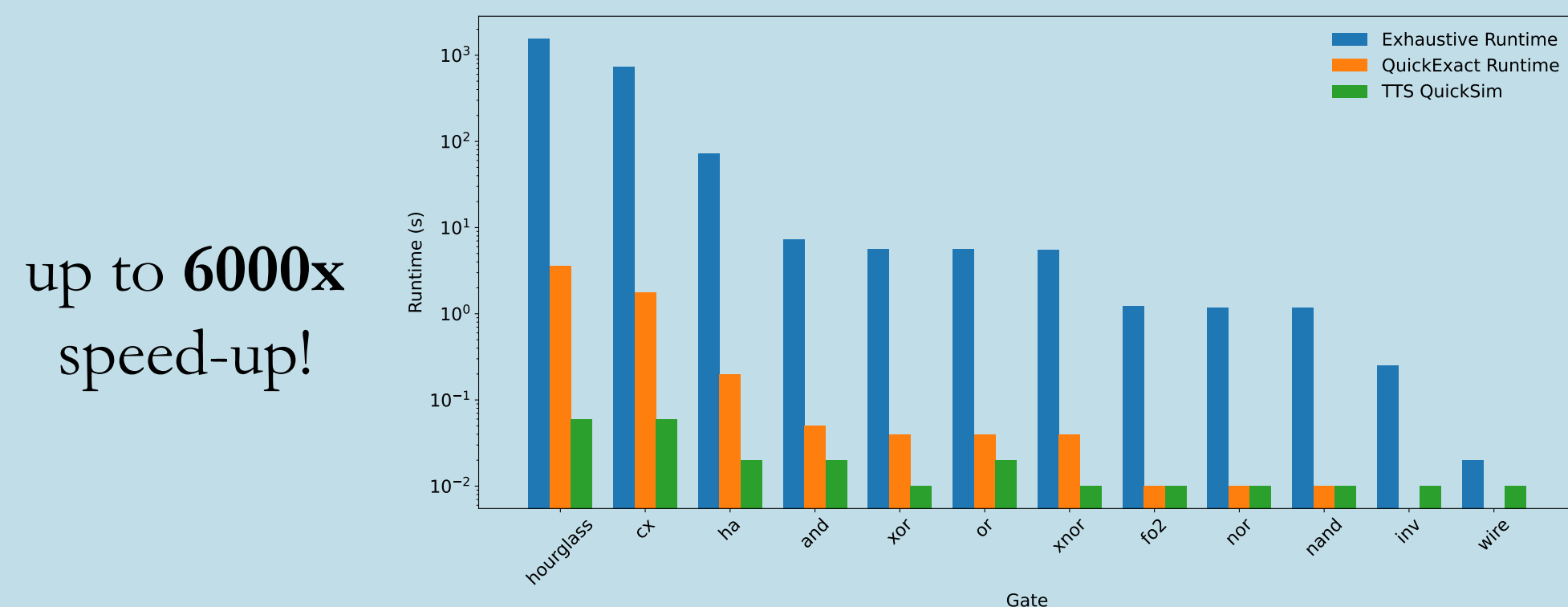
- Designing and simulating atomic-scale computing.
- Multiple levels of abstraction are addressed, namely
 - Physical Simulation,**
 - Logic Design,**
 - Analysis,**
 - Circuit Design.**
- A **framework** that bridges these gaps by proposing comprehensive design rules and developing **software tools** to facilitate their enforcement.
- Bridging the fields of computer science, electrical engineering, and physics leads to a **holistic design flow**, informed by **fabrication constraints** and driven by **computational strategies**.

Predicting the behavior of SiDB layouts before manufacturing

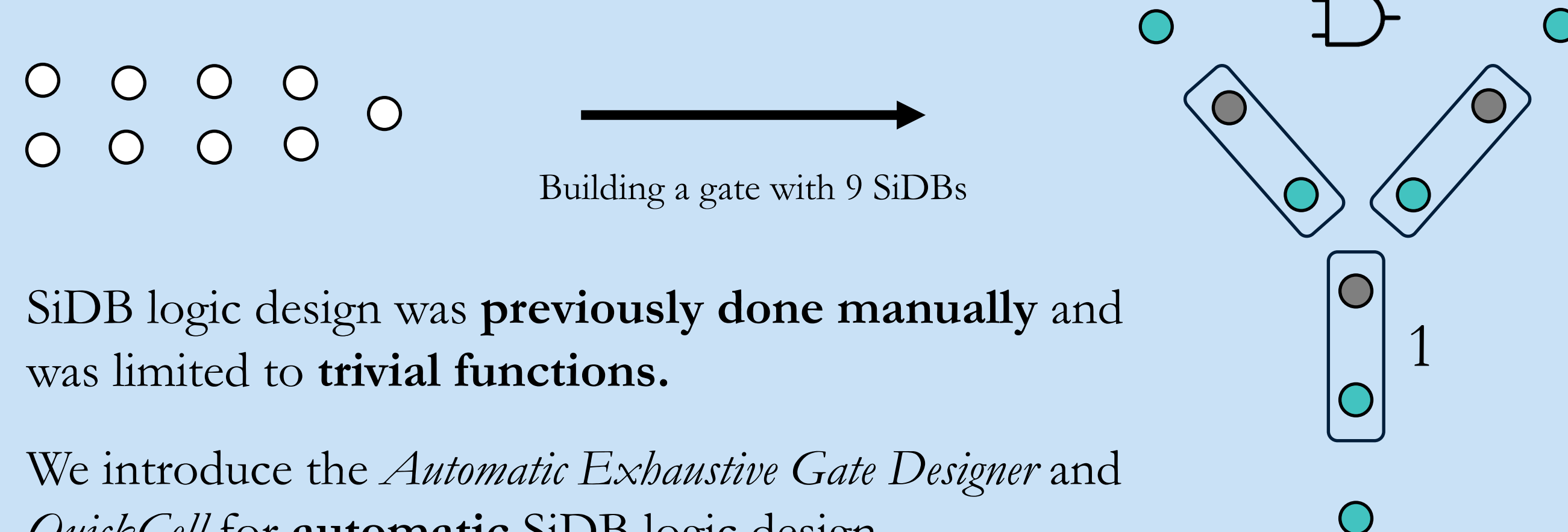


Physical Simulation is an **exponential problem** in the number of SiDBs. Previous solutions were slow, inaccurate, and **limited to small layouts**.

We introduce *QuickSim* and *QuickExact*, innovative physical simulators that integrate principles of **physics and computer science**.

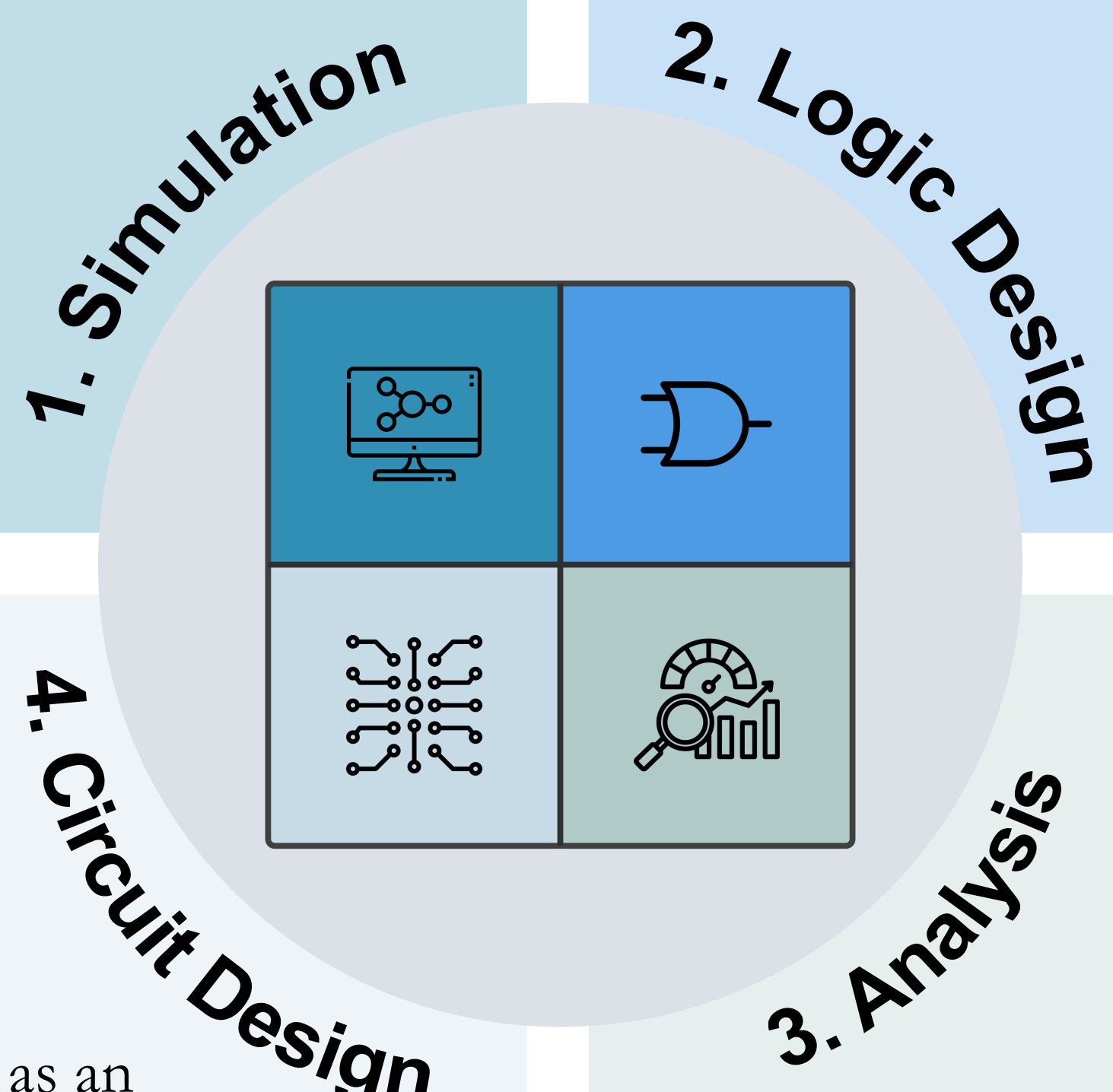


Arranging SiDBs to realize logic



SiDB logic design was **previously done manually** and was limited to **trivial functions**.

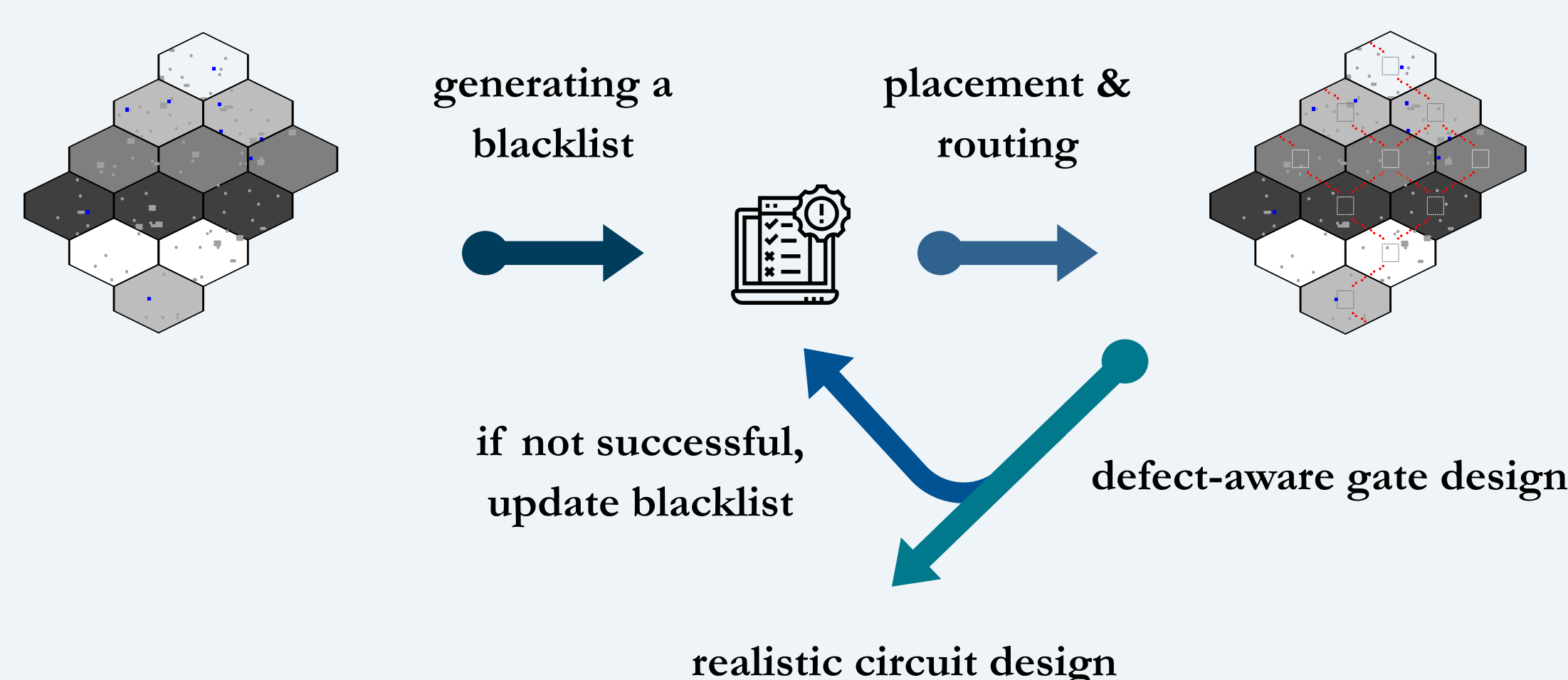
We introduce the *Automatic Exhaustive Gate Designer* and *QuickCell* for **automatic** SiDB logic design.



Designing SiDB circuits

Atomic defects are prevalent on SiDB substrates and **disturb logic operation**.

Atomic defects are integrated into the layouts of logic gates as an integral part of the gate-level layout design as well as gate design. The result is an SiDB circuit that **works on a defective surface**.

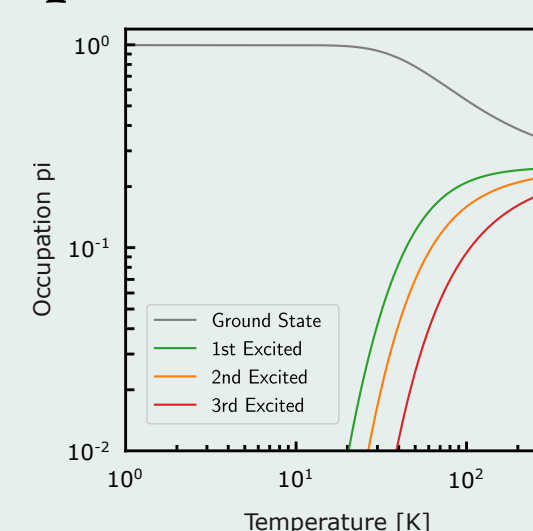


Performing analysis of SiDB logic

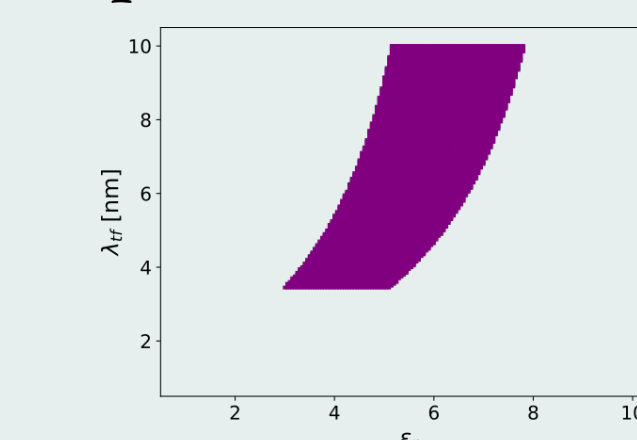
Insufficient methodologies for analyzing SiDB logic.

Multiple analysis methodologies and algorithms are established to **assess the robustness of SiDB logic**.

Temperature Simulation



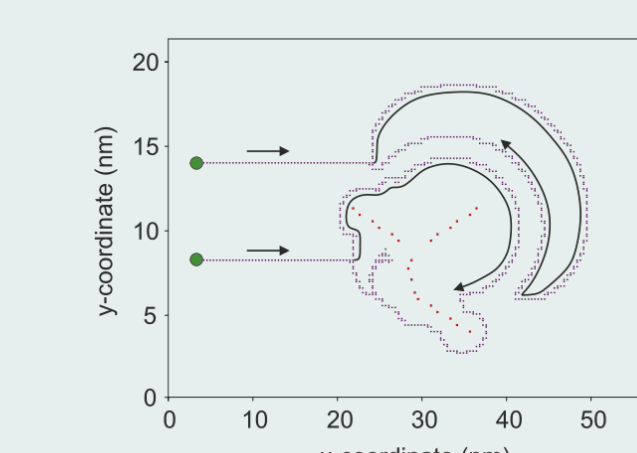
Operational Domain



Cost Function for SiDB Logic

Systematic approach to designing SiDB logic that optimize across multiple figures of merit.

Defect Robustness



Open-Source Projects



Publications

- 12 Publications
 - 2x Design Automation Conferences (ASP-DAC and DATE)
 - 2x ACM International Symposium on Nanoscale Architectures (Nanoarch)
 - 7x IEEE International Conference on Nanotechnology (IEEE Nano)
 - 1x ISCAS 2025.
- 7 papers are under review at TCAD, ICCAD 2025, NANO 2025, DAC 2025.

Collaborations

- A collaboration was established with international researchers from the **University of Alberta** (physicists, hardware engineers) and the **University of British Columbia** (electrical engineers) in Canada, leading to 7 papers.
- An intensive collaboration with *Quantum Silicon Inc.* was initiated, which included a research exchange in Canada supported by the Bavarian Research Alliance (BayFOR).
- The presented physical simulators have been integrated into the CAD tool *SiQAD*, showcasing the recognition of our work.