# Executive Summary

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## Introduction

From modeling and simulation point of view the main issue related to the simulation of devices with precisely placed dopants is the resolution of the impact of the individual discrete dopants on the device characteristics using different simulation techniques. The problem is exacerbate by the necessity to use 3D simulations when resolving the individual discrete dopants and the corresponding needs of significant computing power. In the recent years steady progress have been made in resolving individual discrete dopants in drift diffusion (DD), Monte Carlo (MC) and quantum transport simulation tolls (QT). Capabilities to resolve individual discrete dopants in DD, MC and QT transport simulation tools is essential when developing concepts for nanoelectronic devices that can benefit from the accurate placement of individual discrete dopants. Of course this should be supplemented by fist principle simulation techniques, which are needed to understand the physics and interactions between dopants and the crystal lattice and to validate, calibrate and parameterize the DD, MC and QT simulation techniques

## The progress of selected topics over the past five years including your results

**DD simulations**

The introduction of density gradient quantum corrections for both electrons and holes has resolved the problem of artificial charge trapping in the coulomb well of the attractive potential of ionized impurities. This has removed the mesh sensitivity associated with the singular coulomb potential of individual dopants. This is the most physical and accurate way of resolving individual discrete dopants in DD simulations.

**MC Simulations**

The introduction of ab-initio impurity scattering has allowed transport variation related to individual dopant positions to be captured in 3D ensemble MC simulations. This is essential when resolving the impact of individual dopants on the current and the performance of nanoelectronic devices. Please note that DD simulations capture accurately the impact of individual dopants on the device electrostatics and provide acurate results in the subthreshold region but currently cannot resolve the impact of individual dopants on the on-current.

**QT Simulations**

Full 3D QT simulators are now readily available. Both effective mass and Tight Binding Hamiltonians are used. Recently discrete dopants were successfully introduced in such simulators. The preferred approach is the Nonequilibrium Green's Functions (NEGF) approach that can facilitate the introduction of scattering in QT simulations. Currently the main focus of

## Potential application opportunities, if possible (What is the potential impact on ITRS?)

The main application domain for DD, MC and QT simulation tools that can resolve individual discrete dopants is in the simulation and study of statistical variability in conventional and novel MOSFET architectures essential for the More Moore domain. This includes bulk, FD SOI, FinFETs and nanowire (gate all around) MOSFETs. The important question to answer here include to what extend the accurate placement of individual dopants:

- Can improve the variability, bearing in mind their interactions with other variability sources;
- To what extend the placement accuracy affects the variability.

Another important domain is the improvement of device performance by accurate dopants placement. The important questions to answer include what extend the precise placement of individual dopants:

- Can reduce the contact resistance;
- Can reduce the resistance of the source/drain regions;
- Can improve short channel effects including subthreshold slope and DIBL;
- Can increase mobility and injection velocity and reduce backscattering.

Simulations that capture the impact of individual dopants will be very important in the Beyon Moore domain where the interactions between precisely positioned dopants can enable new computing paradigms including quantum computing.

Finally simulations that capture individual dopants can serve the More than Mooor domain particularly in sensory applications using single electron transistors MOSFETs tailored to read the charge distribution of molecules. One



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example is the DNA sequencing.

The difficult challenges and potential solutions for the next 10 – 15 years

**DD simulations**

- Computational efficiency.
- Mobility models that reflect the impact of individual dopants on the transport and therefore on the on-current and performance.

**MC Simulations**

- Computational efficiency.
- Efficient short-range corrections for the impurity potential and the short range driving force.
- Impact of the interface on the short-range corrections and driving force.
- Efficient techniques for self force avoidance.

**QT Simulations**

- Computational efficiency.
- Accurate resolution of the impurity potential.
- Efficient introduction of phonon and surface roughness scattering.
- Coupling to heat flow.
- Coupling to first principle DFT simulations.

One very important challenge is the development of truly multi-scale simulation approach that can apply different simulation techniques in different regions of the simulated device and the environment. This will allow all relevant effects to be captured in efficient manner. This is also essential for a meaningfull comparison between the simulation data and the experimental measurements.

Experts and expertise with references

The essential references below are focused on resolving individual discrete dopants in DD, MC and QT simulations. The lead expert is underlined.

**DD simulations**

N. Sano, K. Matsuzawa, M. Mukai, and N. Nakayama, "On discrete random dopant modelling in drift-diffusion simulations: Physical meaning of 'atomistic' dopants," Microelectron. Reliab., vol. 42, no. 2, pp. 189–199, Feb. 2002.

G. Roy, A. R. Brown, F. Adamu-Lema, S. Roy and A. Asenov, Simulation Study of Individual and Combined Sources of Intrinsic Parameter Fluctuations in Conventional Nano-MOSFETs, IEEE Trans Electron Dev. Vol. 52, pp. 3063-3070 (2006)

**MC simulations**

C. Alexander, G. Roy, A. Asenov, Random dopant induced drain current variation in nano-MOSFETs: A tree dimensional self-consistent Monte Carlo study using 'ab-initio' ionized impurity scattering, IEEE Trans. Electron Dev. Vol. 55, No 11, pp 3251-3258 (2008).

W. J. Gross, D. Vasileska and D. K. Ferry "A Novel Approach for Introducing the Electron-Electron and Electron-Impurity Interactions in Particle-Based Simulations", IEEE Elec. Dev. Lett., 20, pp.463-465, 1999.

C. J. Wordelman and U. Ravaioli "Integration of a Particle-Particle-Particle-Mesh Algorithm with the Ensemble Monte Carlo Method for the Simulation of Ultra-Small Semiconductor Devices" IEEE Trans. Elec. Dev., 47, pp.410-416, 2000.

P. Dollfus, A. Bournel, S. Galdin, S. Barraud and P. Hesto, "Effect of Discrete Impurities on Electron Transport in Ultrashort MOSFETs Using 3-D MC Simulation" IEEE Trans. Elec. Dev., 51, pp.749-756, 2004.

**QT simulations**

A. Martinez, J.R. Barker, A. Svizhenko, M.P. Anantram, and A. Asenov, The impact of random dopant aggregation in source and drain on the performance of ballistic DG nano-MOSFETs: A NEGF study, IEEE Trans. Nanotechnology, Vol. 6, No. 4 pp. 438-445 (2007).

M. Luisier, A. Schenk, and W. Fichtner," Quantum transport in two- and three-dimensional nanoscale transistors: Coupled mode effects in the nonequilibrium Green's function formalism, J. Appl. Phys. 100, 043713 (2006).

R. Lake, G. Klimeck, R. C. Bowen and D. Jovanovic, "Single and multiband modeling of quantum electron transport through layered semiconductor devices", J. App. Phys., Vol.81, p.7845 (1997).



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