

# International Workshop on Computational Nanotechnology

## Transport through Si QDs in coulomb blockade regime: Theory and experiment

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The aim of this work is to develop a theory that can predict the transport through quantum dots (QDs) in the Coulomb blockade regime without any adjustable parameters, which will allow to use this model as a design tool for new structure with predefined properties for quantum computing applications. We present a detailed 3D modelling of transport through Si QD single electron transistor used for charge sensing in the devices for quantum information applications. For this reason we are only interested in the relative change of the current and not the absolute values. This means that we do not need to calculate the tunnelling rates and the relative change of the current (so-called stability diagrams – the current as a function of two gate voltages) can be calculated using the effective capacitance matrix approach that we have developed. The model includes several stages: 3D digitization of the real QD device (see Fig.1); electron wavefunction calculations in the QDs through the solution of the coupled Poisson's and Schroedinger-like equations; determination of the effective capacitance matrix of the device; transport calculations in the Coulomb blockade regime using the solution of the master equations. We apply the developed model to two types of the devices. The first type includes the structures [1] with trench-isolated double QDs and single electron transistors (formed as source, drain and side gates and the QD, see bottom of left image in Fig.1). The second type includes the structures with silicon nanowire field-effect transistors [2] with corner QDs formed by the electric field in the channel of the transistor. In both cases we have built a real 3D device and carried out the modelling of the transistor current to compare with the experiment [1,2]. It is important to note that the model does not contain any adjustable or fitting parameters – using the device structure and geometry we were able to predict qualitatively and quantitatively the current variations in both types of devices and reproduce stability diagrams showing charge movements in the QDs observed in experiment [1,2]. We conclude that the developed model can be used as a design and optimisation tool for new structures and predicting new phenomena for quantum information applications. This work is partly financially supported by Kakenhi Grants-in-Aid (Nos. 26709023 and 26249048) and JST-CREST, and by the European Community's Horizon 2020 Programme (Grant Agreement No. 688539).

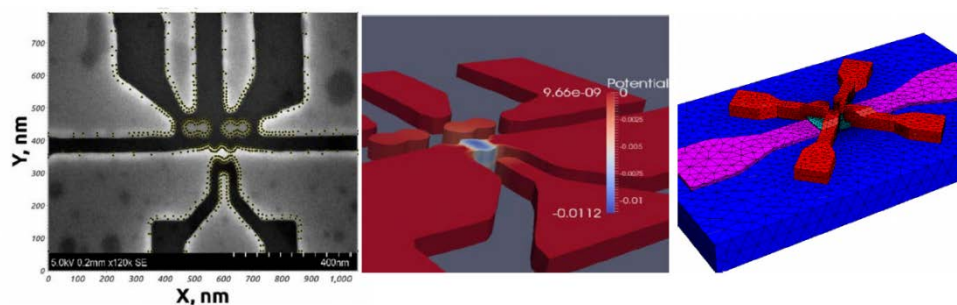


Fig.1 (left): SEM image of the structure with Si isolated double QDs and single electron transistor; the dots show the digitisation of the structure used for the modelling; (middle): calculated 3D distribution of electrical potential in the structure on the left as part of effective capacitance determination for Coulomb blockade transport modelling; (right): 3D model image of the structure with silicon nanowire field-effect transistor with 4 gates and QDs used for the modelling.

- [1] T.-Y. Yang, et.al., 2016 IEEE International Electron Devices Meeting (IEDM), (2016) [2] M.F. Gonzalez-Zalba, et.al. Nature Comm. 6, 6084 (2015)
- [2] M.F. Gonzalez-Zalba, et.al. Nature Comm. 6, 6084 (2015)