Large dangling bond electronic circuits with the supporting surface and contacting nano-pads.

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Electron transport through a very large dangling bond circuit interconnected using many nano-pads (see the circuit below), can be calculated using the N-ESQC technique [1] in its semi-empirical version. The corresponding multi-electrode multi-channel scattering matrix is calculated taking into account the full valence electronic structure of the supporting surface, the metallic interconnection nano-pads and the dangling bond circuit. The electronic band structure of the Si(100)H supporting surface together with the one of the atomic wires are presented looking at their dependence on the number of layers describing the surface. The through surface leakage current between the nano-pads is analyzed [2]. The N-ESQC technique will be compared with other methods based on DFT or simply tight binding approaches when applied to those large surface circuits. The scalability of the required computer memory and computational time are discussed as a function of the size of the system.

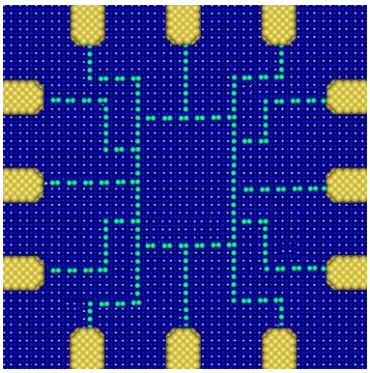

Figure: Example of a 12 interconnection nano-pads dangling bond circuit constructed on a Si(100)H surface.

References:

[1] S. Ami and C. Joachim, Phys. Rev. B 65 (2002) 115419.

[2] F. Ample, I. Duchemin, M. Hliwa and C. Joachim, J. Phys. CM, 23 (2001) 125303.