Institut Ruđer Bošković
ZAVOD ZA TEORIJSKU FIZIKU
Bijenička c. 54
Zagreb, Hrvatska

SEMINAR ZAVODA ZA TEORIJSKU FIZIKU

(Zajednički seminari Zavoda za teorijsku fiziku,
Zavoda za eksperimentalnu fiziku IRB-a i Fizičkog odsjeka PMF-a)

Modeling interfaces and surfaces using density functional theory and nonequilibrium Green's function method

U. Martinez
Quantum Wise A/S, Copenhagen

Datum: utorak, 7. ožujka 2017.
Vrijeme : **15:30 sati c.t.**
Mjesto: IRB, predavaona I krila

Abstract:

This talk will highlight some of the unique features of Atomistix ToolKit and Virtual NanoLab [1] software relevant for simulation of interfaces in general, and metalsemiconductor interfaces in particular. Nonequilibrium Greens function formalism is used to describe the electronic transport properties of such structures. This methods includes all the relevant ingredients required to model realistic metalsemiconductor interfaces and allows for a direct comparison between theory and experiments via IV bias curve simulations [2], for example. Finally, the new oneprobe configuration for reliable simulations of surfaces is also introduced. The central difference to traditional slab calculations is that the surface electronic structure is coupled to the bulk electronic structure through the nonequilibrium Greens function (NEGF) method with physically correct boundary conditions.

References

[1] Atomistix ToolKit version 2016.4, QuantumWise A/S (www.quantumwise.com).

[2] Stradi D., Martinez U., Blom A., Brandbyge M., and Stokbro K. Phys. Rev. B 93, 155302 (2016)

Voditelj seminara:
Andjelo Samsarov
$\langle asamsarov@irb.hr \rangle$