

Topic PhD QT: Theoretical study of charge transfer in nanostructures

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Abstract: Nanotechnology is one of the key science disciplines that will fundamentally influence the development of our society. One of the promising directions of nanotechnology is linked to the possibility of charge and spin control on the atomic scale. The possibility of actively controlling atomic-level charge transfer in nanostructures opens up new possibilities in the field of nanoelectronics. A deeper understanding of the processes involved in charge transfer at the atomic level requires new procedures in the field of theoretical simulations.

Within the doctoral study the student will acquire basic theoretical methods for computer simulations of electron and atomic structures of nanostructures on the surface of solid matter. Student will acquire theoretical backgrounds of scanning microscopy and charge transport at atomic level. In particular, he/she will learn the computational methods associated with the theory of functional density and its application to selected problems of the charge transfer in nanostructures.

The aim of the thesis is to study selected problems of description of nanostructures on solid surfaces and their physical and chemical properties using numerical simulations. The calculations will be carried out in close cooperation with experimental measurements. Further development of computer simulations is also envisaged in doctoral studies.

References:

[1] R.M. Martin, Electronic structure: Basic Theory and Practical Methods, Cambridge University Press, 2004.

[2] W. Koch, M.C. Holthausen, A chemist's Guide to Density Functional Theory, Wiley-VCH, 2001.