

# Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensed Matter Physics of Charles University has a pleasure to invite you to attend the seminar

**on 5 December 2019 at 14:00**

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

**Lecture hall F2**



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## Toward Automatic Interpretation of submolecular AFM images

Joined with Nanoseminar. Note different time and place.

In recent decade Atomic Force Microscopy with tip functionalized by carbon monoxide (CO) provided unique tool to experimentally image sub-molecular details of individual organic molecules [1]. In principle it allows to map distribution of electron density and electrostatic potential, which is of great importance e.g. for on-surface chemistry. Direct interpretation of the images is however complicated by convolution of electric fields and strong relaxation of CO molecule causing severe image distortions. This problem can be partially overcome by simple mechanical model (Probe-Particle Model [2]) which can reproduce these effects, therefore simulate AFM images for given molecular structure. However, this still requires laborious search for molecular structure which reproduces that particular experimental image. Instead we attempt to develop automatic tool to conduct inverse task – to recover molecular structure from given set of AFM images. Our result shows that convolution neural network (CNN) [3] trained on simulated AFM images can learn this inverse mapping at least for simulated images. One of the challenges in order to achieve reliable results on experimental data is synthesis of sufficient amount of realistic training examples at feasible computational cost.

[1] Gross, L., Mohn, F., Moll, N., Liljeroth, P., Meyer, G.; The chemical structure of a molecule resolved by atomic force microscopy, *Science*, 325(5944), 1110–1114 (2009).

[2] Hapala, P., Kichin, G., Wagner, C., Tautz, F. S., Temirov, R., Jelínek, P. *Phys. Rev. B*, 90(8), 085421 (2014).

[3] Lecun, Y., Bottou, L., Bengio, Y., Haffner, P.; *Proceedings of the IEEE*, 86(11), 2278–2324 (1998).

