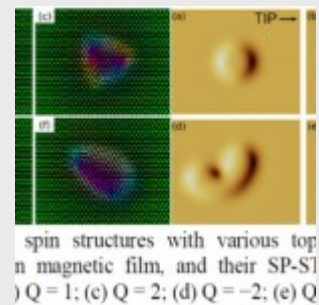


## Complex Magnetic Structures at Surfaces and Their Imaging with STM from First Principles



Title: Complex Magnetic Structures at Surfaces and Their Imaging with STM from First Principles.

When: Monday, June 12, (2017), 12:00.

Place: Departamento de Física Teórica de la Materia Condensada, Facultad Ciencias, Module 5, Seminar Room (5th Floor).

Speaker: Krisztián Palotás, Department of Complex Physical Systems, Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia.

**R**ecent advances in spin-polarized scanning tunneling microscopy (STM) experiments allow the determination of complex (non-collinear) surface magnetic structures (like spin-spirals, skyrmions) in real space. Motivated by these advancements, there is a strong need for theoretical understanding of the observed magnetic structures. In the first part of the talk I present recent theoretical results on the formation of a diversity of complex magnetic structures in thin films obtained by a combination of ab initio and spin dynamics calculations [1].

Understanding STM image contrasts is of crucial importance in surface science and related technologies. In the second part of the talk I present various STM theories and highlight different tip effects on the STM contrast based on first principles calculations, going beyond the Tersoff-Hamann model, e.g., within 3D-WKB tunneling theory [2]. Examples include a prototype frustrated hexagonal antiferromagnet, Cr monolayer on Ag(111) [3], metastable skyrmionic structures with various topologies [4] and highly oriented pyrolytic graphite. By comparing STM topographic data between experiment and large scale simulations, we can determine particular tip orientations that are most/least likely present in the STM experiment [5]. Furthermore, I present an extension of Chen's derivative rule for STM simulations including tip-orbital interference effects, and demonstrate the importance of such effects on the STM contrast for two surface structures: N-doped graphene and a magnetic Mn<sub>2</sub>H complex on the Ag(111) surface [6]. Finally, the first steps towards the theoretical modeling of high resolution spin transfer torque imaging are presented [7].

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