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SIMULATION OF SPIN-POLARIZED SCANNING TUNNELING MICROSCOPY AND SPECTROSCOPY ON MAGNETIC SURFACES

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DATE / TIME	16.01.2012, 04:00 p.m. (CET)
LOCATION	Seminar Room 138C, Vienna University of Technology, "Freihaus"-building, 9th floor, "yellow" – Wiedner Hauptstraße 8-10, A-1040 Vienna, AUSTRIA)

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In this talk, a computationally cheap and flexible atom-superposition-based method for simulating spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy (SP-STS) is presented. The approach is based on the spin-polarized Tersoff-Hamann model and the Wentzel-Kramers-Brillouin approximation, and its main advance is the inclusion of the tip electronic structure. The method is fast as it is easy to parallelize, and it is flexible as it can be combined with any ab initio electronic structure code.

Using this method, we study how the tip magnetization and electronic structure affects the differential conductance (dI/dV) tunneling spectrum of an Fe(001) surface [1]. Our results suggest that the sensitivity of SP-STS on a magnetic sample can be tuned and even enhanced by choosing the appropriate magnetic tip, and the effect is governed by the effective spin polarization.

Integrating the differential current contributions in an energy window corresponding to the applied bias voltage, SP-STM can be simulated in high spatial resolution [2]. The capabilities of the method are illustrated for a complex magnetic surface, the prototype frustrated hexagonal antiferromagnet, Cr monolayer on Ag(111) in a noncollinear magnetic 120 degrees Néel state. We find that the magnetic contrast is sensitive to the tip electronic structure, and this contrast can be reversed depending on the bias voltage [2]. Moreover, we demonstrate that the dI/dV can be calculated directly, without numerical differentiation of the tunneling current, and we analyze the contributing terms to the differential conductance. The effect of the tip electronic structure on the tunneling spectra and the related magnetic asymmetries are also highlighted.

References: [1] K. Palotás, W. A. Hofer, and L. Szunyogh: "Theoretical study of the role of the tip in enhancing the sensitivity of differential conductance tunneling spectroscopy on magnetic surfaces", Phys. Rev. B 83, 214410 (2011). [2] K. Palotás, W. A. Hofer, and L. Szunyogh: "Simulation of spin-polarized scanning tunneling microscopy on complex magnetic surfaces: Case of a Cr monolayer on Ag(111)", Phys. Rev. B 84, 174428 (2011).

Acknowledgments: Financial support of the Magyary Foundation, EEA and Norway Grants, the Hungarian Scientific Research Fund (OTKA) (Project IDs: PD83353, K77771), the Bolyai Research Grant of the Hungarian Academy of Sciences, and the New Széchenyi Plan of Hungary (Project ID: TÁMOP-4.2.1/B-09/1/KMR-2010-0002) is gratefully acknowledged.