

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)

Magnetic Properties of Hybrid Organic-Metal Interfaces

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Datum: utorak, 24. lipnja 2014.
Vrijeme : **11:00 sati c.t.**
Mjesto: IRB, dvorana I krila

Abstract:

In order to construct functional organic-based electronic components in organic electronic and spintronic devices it is essential to gain a fundamental theoretical understanding of the organic-electrode interface. The density functional theory provides a framework with predictive power where a realistic description of these organic-metal hybrid systems can be expected. I will present theoretical studies that explain how the subtle interplay between the chemical, electrostatic and the weak van der Waals adsorption mechanisms determines the geometry, electronic and magnetic structure of organic-metal interfaces. Such first-principles calculations are applied to unravel the electronic and magnetic properties of the adsorbed organic material on surfaces and can provide not only the basic insights needed to interpret surface-science experiments but are also a key tool to design organic-substrate systems with tailored properties that can be integrated in organic-based devices.

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