NanoLab Talk

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Seminar Room 1° floor

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Organic molecules at surfaces: insight from theoretical core-level spectroscopy

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An adsorbed organic molecule or a thin overlayers constitute the paradigmatic building block in the description of hybrid interfaces bearing key role in various technological applications. Surface-science techniques based on core-level spectroscopy can provide important information about their properties, especially when experimental and theoretical analysis are combined. In this talk I will consider two closely related techniques, presenting theoretical methods and discussing examples.

Near-edge X-ray absorption fine structure (NEXAFS) accesses molecular orientations and provides information on the unoccupied electronic levels. I will present an extension of it analysis from the standard case of planar polycyclic aromatic hydrocarbons to curved molecules such as buckybowl corannulene [1], and to systems including sp^1 C chains [2], with simple transition-potential approximation already capable to capture the main physical aspects.

Resonant photoemission spectroscopies (RESPES) can measure interfacial electron transfer times down to the femtosecond timescale, yet with a significant distortion given the presence of the core-hole. I will show that room-temperature estimates for molecules on TiO_2(110) may be obtained through accurate sampling of the molecular trajectories [3], and that buffer graphene layers can decouple organic/graphene/metal interfaces [4].

References

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About the speaker:

Guido Fratesi is fixed-term researcher at the University of Milan since 2013. He has obtained the Ph.D. in theoretical condensed matter physics at S.I.S.S.A. in 2005 with a thesis on heterogeneous catalysis modeling. He then performed post-doctoral research at the University of Milano-Bicocca and the University of Milan. His interests are in the ab initio description of the properties of surfaces and adsorbed systems, especially molecules and low-dimensional materials at crystal surfaces.

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