

Theoretical investigations of the structure and dynamics of surfaces and adlayers

*Branko Gumhalter^{*1}, Predrag Lazić², Radovan Brako²,
Željko Crljen², Antonio Šiber¹, Damir Aumiler¹, Hrvoje Buljan³*

¹Institute of Physics, ²Ruđer Bošković Institute, ³Faculty of Science, Zagreb, Croatia

Abstract: This talk reviews several aspects and achievements of the investigations of structural and dynamical properties of surfaces and adlayers undertaken by the members of the local surface science community. Parts of this work have been carried out in collaboration with groups from other countries including Japan. It is envisaged that this line of research may rouse interest and provide a basis for future Croatian-Japanese collaboration in surface science.

The first part of the talk will illustrate results of the endeavours to implement the recently proposed exchange-correlation functionals in the DFT-based calculations incorporating the long range correlations that give rise to van der Waals interactions. The latter are indispensable for the stabilization of weakly bound surface structures and inclusion of their effects enables realistic modelling of vibrational dynamics [1,2,3].

The second part of the talk focuses on the manifestations of various aspects of ultrafast electron dynamics typically encountered in time-resolved electron spectroscopies of surfaces. Particular attention is paid to the interpretations of time resolved experiments in the regimes in which the deviations from standard adiabatic descriptions of the dynamics of investigated systems is expected. The understanding of these deviations and temporal intervals in which they may occur are prerequisites for correct interpretation of a whole menagerie of scientifically important and technically relevant dynamical processes at surfaces [3,4].

(*) Email: branko@ifs.hr; <http://gumhalter.ifs.hr/>

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