ecoss 33
27 AUG – 1 SEP 2017
SZEGED, HUNGARY
33RD EUROPEAN CONFERENCE ON SURFACE SCIENCE

ILLUMINATING NANOSYSTEMS AT SURFACES

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We are now used to consider first principles theories and simulations as reliable and predictive tools for many ground state problems in surface science. Describing excitations and their dynamics from first principles is much tougher, but extremely important to understand fundamental processes following e.g. photoexcitation, and for the theory of spectroscopies. I will present recent progress showing that we are now reaching predictivity and quantitative accuracy for realistic systems also in that case. I will focus on two case studies that we have recently explored: - organic photovoltaic interfaces and model photosynthetic systems [1]: what controls the ultrafast charge separation processes after exciton generation ? - graphene-based nanosystems at surfaces [2]: what is the role of screening and substrate effects on manybody interactions and exciton binding ? what are the excitonic spectral signatures, and how can they help in understanding the self-assembly process at surfaces [2] ? how to identify plasmonic signatures [3]? - In both cases, ab-initio approaches beyond mean-field theories are needed. We use real-time time-dependent density functional theory when coupling to vibrations is critical for large systems, and many body perturbation theory in the GW and Bethe-Salpeter approaches when we need the highest accuracy in excitonic effects. I will discuss how these approaches are helping us to address the above questions and have contributed to successful interpretation of experiments [1-2], and the challenges we see for the future.

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* In collaboration with C. Cardoso, A. Ferretti, D. Prezzi, C.A. Rozzi, A. Ruini, D. Varsano. Computational developments are supported by the European Center for HPC applications 'MaX – materials ate the exascale': www.max-centre.eu.

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